EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
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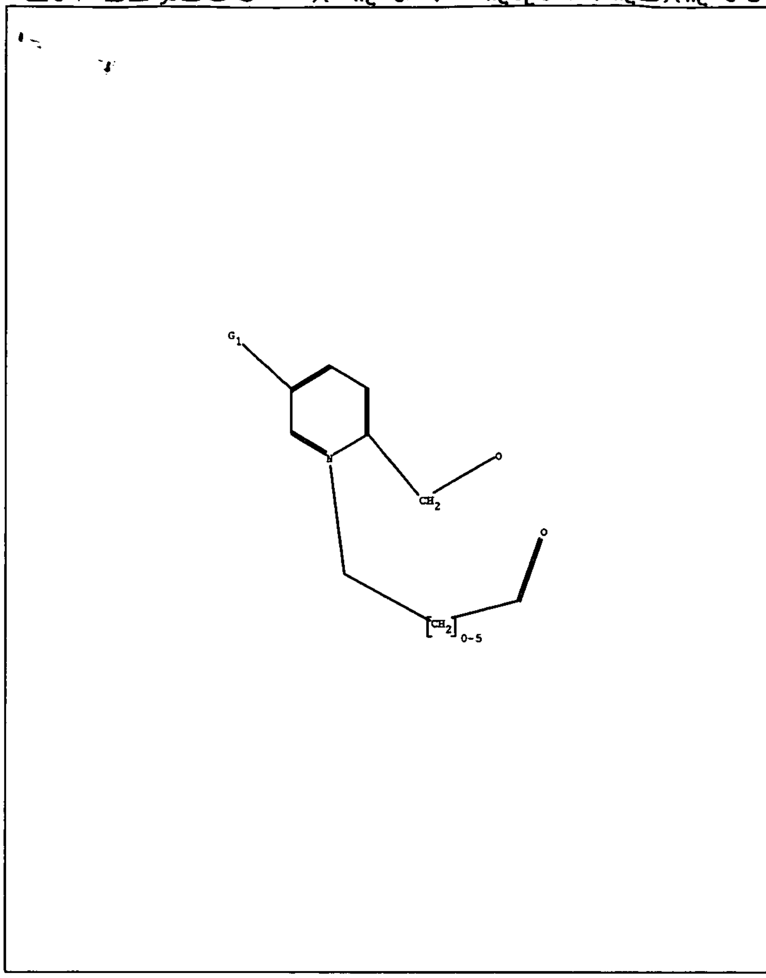

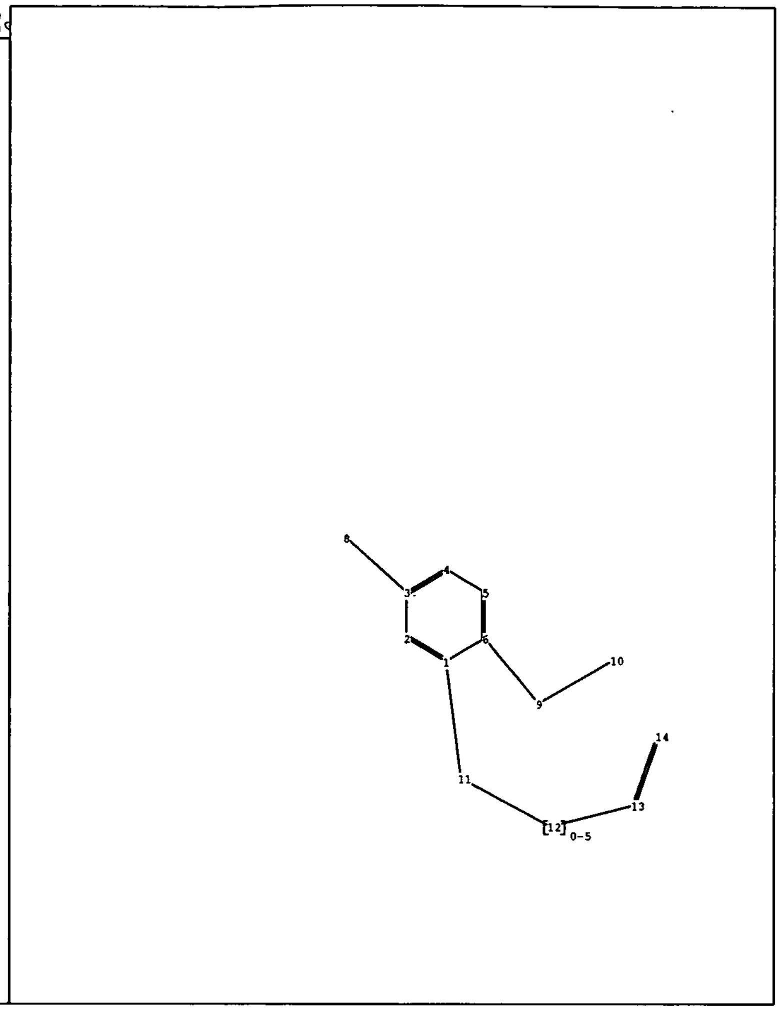

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ring nodes :
1 2 3 4 5 6
chain bonds :
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ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
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exact bonds :
6-9 9-10 11-12 12-13
normalized bonds :
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isolated ring systems :
containing 1 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS
9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS

```
=> d his

     (FILE 'HOME' ENTERED AT 13:51:50 ON 10 MAY 2006)

     FILE 'REGISTRY' ENTERED AT 13:52:13 ON 10 MAY 2006
L1             STRUCTURE UPLOADED
L2               1 S L1
L3              17 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 13:54:19 ON 10 MAY 2006
L4               9 S L3
L5               9 S L4 AND HOFMANN, T?/AU

     FILE 'CAOLD' ENTERED AT 13:56:18 ON 10 MAY 2006

=> s l3
L6               0 L3

=>
```

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	DEC 23	New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/ USPAT2
NEWS 4	JAN 13	IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS 5	JAN 13	New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to INPADOC
NEWS 6	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS 7	JAN 17	IPC 8 in the WPI family of databases including WPIFV
NEWS 8	JAN 30	Saved answer limit increased
NEWS 9	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS 10	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS 11	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS 12	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS 13	FEB 28	MEDLINE/LMEDLINE reload improves functionality
NEWS 14	FEB 28	TOXCENTER reloaded with enhancements
NEWS 15	FEB 28	REGISTRY/ZREGISTRY enhanced with more experimental spectral property data
NEWS 16	MAR 01	INSPEC reloaded and enhanced
NEWS 17	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS 18	MAR 08	X.25 communication option no longer available after June 2006
NEWS 19	MAR 22	EMBASE is now updated on a daily basis
NEWS 20	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS 21	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS 22	APR 04	STN AnaVist $500 visualization usage credit offered
NEWS 23	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 24	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS 25	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS 26	MAY 10	CA/CAplus enhanced with 1900-1906 U.S. patent records

NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT http://download.cas.org/express/v8.0-Discover/

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NEWS LOGIN	Welcome Banner and News Items
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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:51:50 ON 10 MAY 2006

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 13:52:13 ON 10 MAY 2006
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 MAY 2006 HIGHEST RN 883631-57-0
DICTIONARY FILE UPDATES: 9 MAY 2006 HIGHEST RN 883631-57-0

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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Uploading structure

L1      STRUCTURE UPLOADED

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L1                STR
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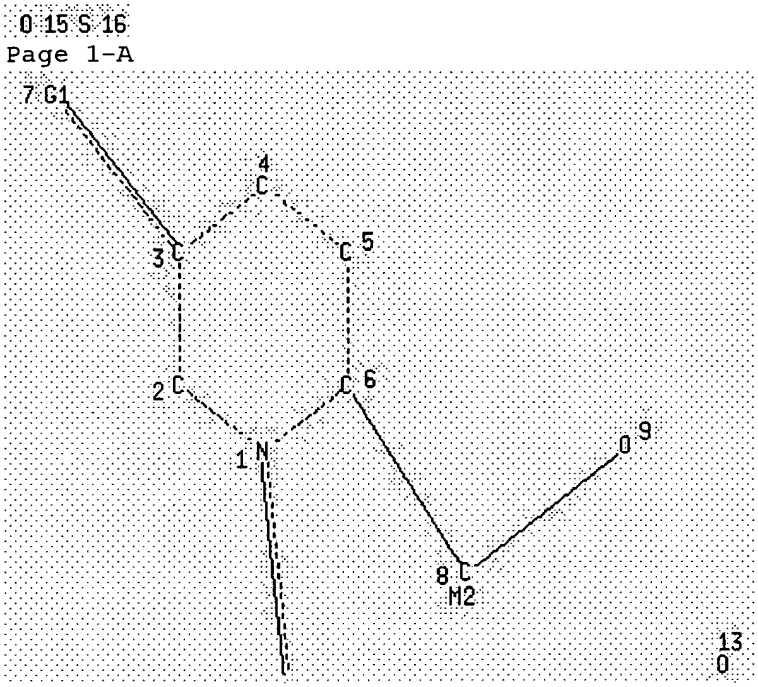
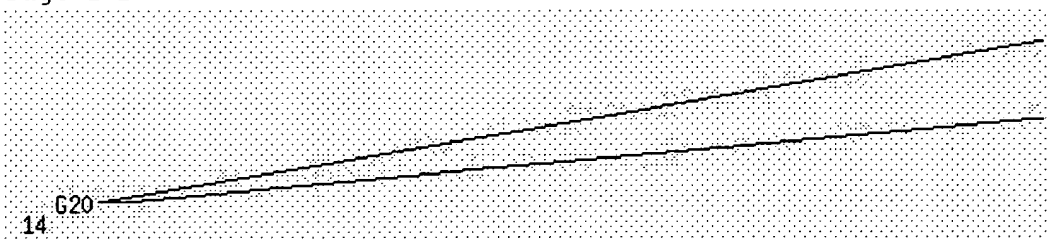
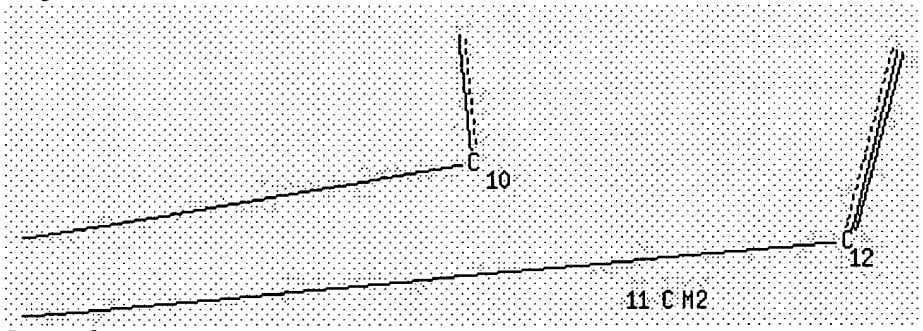


Page 1-B



Page 2-A



Page 2-B

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HCOUNT   IS M2      AT   11
NSPEC    IS R       AT    1
NSPEC    IS R       AT    2
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NSPEC   IS R      AT   4
NSPEC   IS R      AT   5
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NSPEC   IS C      AT   7
NSPEC   IS C      AT   8
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NSPEC   IS C      AT  10
NSPEC   IS C      AT  11
NSPEC   IS C      AT  12
NSPEC   IS C      AT  13
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MLEVEL  IS CLASS  AT   8  9 10 11 12 13 15 16
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  16

STEREO ATTRIBUTES: NONE


=> s l1
SAMPLE SEARCH INITIATED 13:54:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        1 TO ITERATE

100.0% PROCESSED        1 ITERATIONS                              1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            1 TO       80
PROJECTED ANSWERS:               1 TO       80

L2            1 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 166.50 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 13:54:17 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       29 TO ITERATE

100.0% PROCESSED       29 ITERATIONS                             17 ANSWERS
SEARCH TIME: 00.00.01

L3           17 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   168.26     168.47

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FILE LAST UPDATED: 9 May 2006 (20060509/ED)

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=> s l3
L4 9 L3

=> s l4 and hofmann, t?/au
670 HOFMANN, T?/AU
L5 9 L4 AND HOFMANN, T?/AU

=> d l4, ibib abs hitstr, 1-9

L4 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

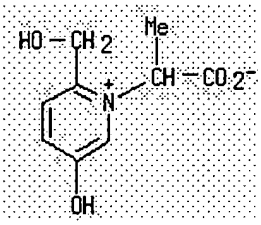
Full Text | Citing References

ACCESSION NUMBER: 2006:354763 HCAPLUS
TITLE: Structural and functional characterization of a multimodal taste enhancer in beef bouillon
AUTHOR(S): Hofmann, Thomas; Soldo, Tomislav; Ottinger, Harald; Frank, Oliver; Robert, Fabien; Blank, Imre
CORPORATE SOURCE: Institut fuer Lebensmittelchemie, Westfaelische Wilhelms-Universitaet, Muenster, D-48149, Germany
SOURCE: ACS Symposium Series (2005), 908(Natural Flavors and Fragrances), 173-188
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review discussing the authors' work on investigating taste enhancers in beef bouillon. Taste activity-guided fractionation combined with the comparative taste diln. anal. led to the discovery of the presence of a sweet enhancing compd. Model Maillard reactions, spectroscopic and synthetic expts. revealed the previously unknown 1-(1-carboxyethyl)-5-hydroxy-2-(hydroxylmethyl)-pyridinium inner salt, named alapyridaine, as the first nonvolatile, tasteless sweet enhancer reported. Sensory anal. of synthetic beef taste reconstitutes spiked with synthetic alapyridaine in its "natural" concn. revealed a significant increase in sweetness, but also in the salty and umami character. Addnl. systematic sensory studies demonstrated for the first time that this compd. is a general taste enhancer which is able to simultaneously intensify sweet, salty and umami taste modalities. Studies on the influence of the stereochem. on sensory activity revealed the (+)-(S)-alapyridaine as the physiol. active compd., whereas the (-)-(R)-enantiomer did not show any effect.

IT **501421-91-6**, Alapyridaine
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(structural and functional characterization of a multimodal taste

enhancer in beef bouillon)
RN 501421-91-6 HCAPLUS
CN Pyridinium, 1-(1-carboxyethyl)-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

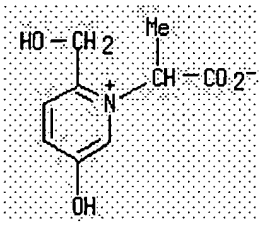
Full Text | Cited References

ACCESSION NUMBER: 2005:1078393 HCAPLUS
DOCUMENT NUMBER: 144:5655
TITLE: Application of hydrophilic interaction liquid chromatography/comparative taste dilution analysis for identification of a bitter inhibitor by a combinatorial approach based on Maillard reaction chemistry
AUTHOR(S): Soldo, Tomislav; Hofmann, Thomas
CORPORATE SOURCE: Deutsche Forschungsanstalt fuer Lebensmittelchemie, Garching, D-85748, Germany
SOURCE: Journal of Agricultural and Food Chemistry (2005), 53(23), 9165-9171
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Activity-directed fractionation of heated carbohydrate/alanine solns. recently led to the discovery of (+)-(S)-1-(1-carboxyethyl)-5-hydroxy-2-(hydroxymethyl)pyridinium inner salt (alapyridaine), and it has been shown that this compd. lowers the detection thresholds of sugars, glutamate, and NaCl solns., whereas no influence on bitter perception was obsd. As this class of Maillard-derived pyridinium betaines seemed to be promising targets for further research on their taste modulatory activity, the objective of the present investigation was to screen for bitter taste-suppressing target mols. in combinatorial libraries of pyridinium betaines prepd. from 5-(hydroxymethyl)furan-2-aldehyde and amino acid mixts. by use of Maillard-type reaction chem. instead of synthesizing and purifying each deriv. individually. By application of hydrophilic interaction liq. chromatog. in combination with the recently developed comparative taste diln. anal., followed by structure detn., synthesis, and sensory studies, we have now succeeded in identifying 1-carboxymethyl-5-hydroxy-2-hydroxymethylpyridinium inner salt (I) as a potential bitter-suppressing candidate. While tasteless on its own, I was found to reduce the bitterness of various bitter tastants such as the amino acid L-phenylalanine, the peptide Gly-Leu, the alkaloid caffeine, and the bitter glycosides salicin and naringin.

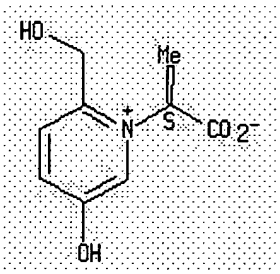
IT 501421-91-6, Alapyridaine
RL: BSU (Biological study, unclassified); FMU (Formation, unclassified); BIOL (Biological study); FORM (Formation, nonpreparative)
(hydrophilic interaction liq. chromatog./comparative taste diln. anal. for identification of bitter inhibitor by combinatorial approach based

on Maillard reaction chem.)
RN 501421-91-6 HCAPLUS
CN Pyridinium, 1-(1-carboxyethyl)-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

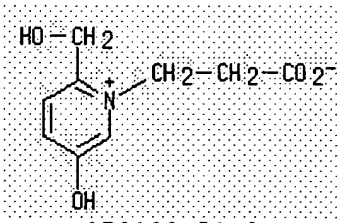


IT **501007-16-5P 870133-50-9P 870133-51-0P**
RL: BSU (Biological study, unclassified); FMU (Formation, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)
(hydrophilic interaction liq. chromatog./comparative taste diln. anal. for identification of bitter inhibitor by combinatorial approach based on Maillard reaction chem.)
RN 501007-16-5 HCAPLUS
CN Pyridinium, 1-[(1S)-1-carboxyethyl]-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 870133-50-9 HCAPLUS
CN Pyridinium, 1-(2-carboxyethyl)-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)



RN 870133-51-0 HCAPLUS
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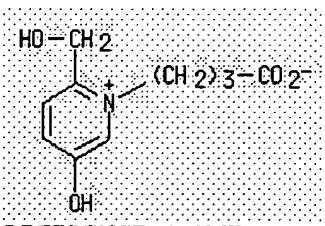


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

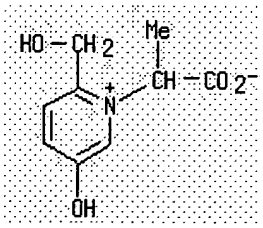
L4 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2005:649868 HCAPLUS
DOCUMENT NUMBER: 144:48527
TITLE: On the relationship between structure and gustatory response of taste enhancing pyridinium betaines
AUTHOR(S): Soldo, T.; Ottinger, H.; Hofmann, T.
CORPORATE SOURCE: German Research Center for Food Chemistry, Garching, 85748, Germany
SOURCE: State-of-the-Art in Flavour Chemistry and Biology, Proceedings of the Wartburg Symposium on Flavour Chemistry and Biology, 7th, Eisenach, Germany, Apr. 21-23, 2004 (2004), 75-80. Editor(s): Hofmann, Thomas; Rothe, Manfred; Schieberle, Peter. Deutsche Forschungsanstalt fuer Lebensmittelchemie: Garching, Germany.
CODEN: 69HCQQ; ISBN: 3-00-015809-X
DOCUMENT TYPE: Conference
LANGUAGE: English

AB Very recently, N-(1-carboxyethyl)-5-hydroxy-2-hydroxymethyl-pyridinium inner salt, named alapyridaine, was identified as a taste enhancing Maillard reaction product inducing a significant increase in human oral sensitivity for sweet tasting sugars and amino acids, for the umami-like tasting mono sodium glutamate as well as for the saltiness of sodium chloride solns. Synthetic studies on the influence of the chem. structure on the human gustatory response of pyridinium betaines revealed that the hydroxyl group and the hydroxymethylene group at position 5 and 2, resp., as well as a (+)-(S)-configured amino acid residue are essential for taste enhancing activity. Depending on the amino acid moiety, some of these pyridinium betaines were found to act as multivalent taste enhancers, whereas others influenced single taste modalities only, or did not impart any bioresponse at all.

IT **501421-91-6**, Alapyridaine
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(hydroxyl group at position 5, hydroxymethylene group at 2, carboxyl, Me group and (S) or (R) amino acid residues were assocd. with gustatory activity of alapyridaine)
RN 501421-91-6 HCAPLUS
CN Pyridinium, 1-(1-carboxyethyl)-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:1039144 HCAPLUS
DOCUMENT NUMBER: 143:171610

TITLE: Systematic studies of structure and physiological activity of alapyridaine. A novel food-born state enhancer

AUTHOR(S): Soldo, Tomislav; Frank, Oliver; Ottinger, Harald; Hofmann, Thomas

CORPORATE SOURCE: Deutsche Forschungsanstalt fuer Lebensmittelchemie, Garching, Germany

SOURCE: Molecular Nutrition & Food Research (2004), 48(4), 270-281
CODEN: MNFRCV; ISSN: 1613-4125

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB By application of taste diln. anal. (+)-(S)-1-(1-carboxyethyl)-5-hydroxy-2-(hydroxymethyl)-pyridinium inner salt was recently successfully identified as a multimodal taste enhancer in beef bouillon. While being taste-less on its own, this so-called alapyridaine was found to intensify the human perception of sweet, salty, and umami taste. To gain information on the mol. requirements of this novel class of taste enhancer, a range of structurally related pyridinium betaines were synthesized, purified, and their physiol. activities sensorially evaluated. Removal or modification of the hydroxyl and the hydroxymethyl group, resp., induced a loss in bioactivity, thus indicating the 2-(hydroxymethyl)-5-hydroxypyridinium moiety as an essential structural element for taste enhancement. Regarding the amino substituent, neither the prolongation or removal of the alkyl chain or the carboxy function in the 1-(1-carboxy-2-ethyl)-moiety, nor the incorporation of an addnl. carboxy function led to any active deriv., thus demonstrating that also the structure of the nitrogen substituent is rather conserved for taste enhancement. But substitution of the Me group by a benzyl group yielded a compd. showing similar taste enhancing activities as found for alapyridaine. Interestingly, addnl. insertion of glycine between the 1-(1-carboxy-2-phenylethyl)-moiety and the pyridinium ring resulted in a compd. eliciting comparable taste enhancing effects as shown for the compd. lacking the glycine spacer. In contrast to these multimodal taste enhancers, substitution of the alanine moiety in alapyridaine by an arginine moiety revealed an one-dimensional taste enhancer exclusively increasing the human sensitivity for salty taste.

IT **861221-38-7P**

RL: BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(systematic studies of structure and physiol. activity of alapyridaine, taste enhancer)

RN 861221-38-7 HCAPLUS

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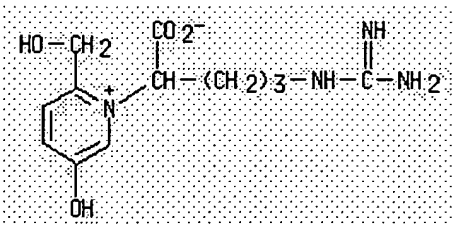


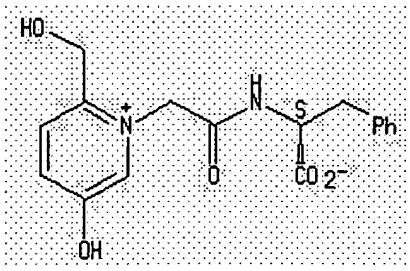
IT **501007-20-1P 861221-32-1P 861221-33-2P 861221-34-3P 861221-35-4P 861221-36-5P 861221-37-6P**

RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic

preparation); BIOL (Biological study); PREP (Preparation)
(systematic studies of structure and physiol. activity of alapyridaine, taste enhancer)

RN 501007-20-1 HCAPLUS
CN Pyridinium, 1-[2-[[(1S)-1-carboxy-2-phenylethyl]amino]-2-oxoethyl]-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 861221-32-1 HCAPLUS
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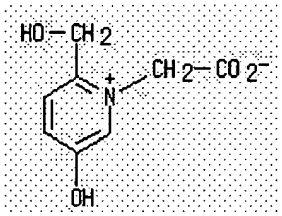

RN 861221-33-2 HCAPLUS
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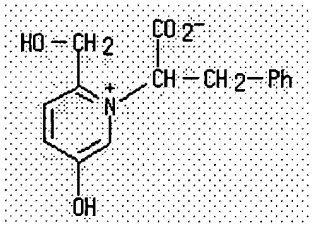
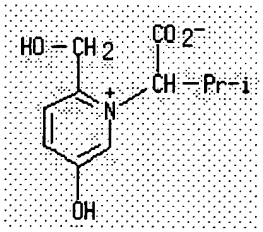
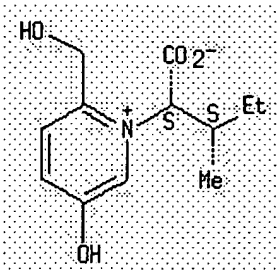


RN 861221-34-3 HCAPLUS
CN Pyridinium, 1-(1-carboxy-2-methylpropyl)-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)



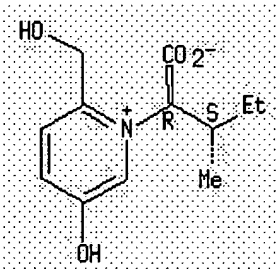
RN 861221-35-4 HCAPLUS
CN Pyridinium, 1-[(1S,2S)-1-carboxy-2-methylbutyl]-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

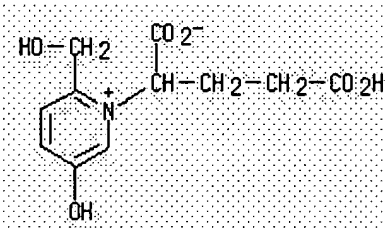


RN 861221-36-5 HCAPLUS
CN Pyridinium, 1-[(1R,2S)-1-carboxy-2-methylbutyl]-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

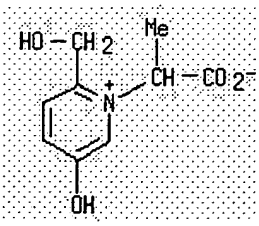
Absolute stereochemistry.



RN 861221-37-6 HCAPLUS
CN Pyridinium, 1-(1,3-dicarboxypropyl)-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)



IT **501421-91-6P**, Alapyridaine
RL: FFD (Food or feed use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(systematic studies of structure and physiol. activity of alapyridaine, taste enhancer)
RN 501421-91-6 HCAPLUS
CN Pyridinium, 1-(1-carboxyethyl)-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

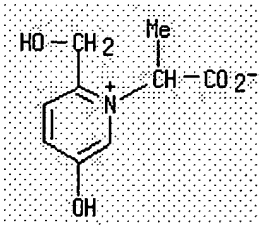
Full Text | Citing References

ACCESSION NUMBER: 2003:765365 HCAPLUS
DOCUMENT NUMBER: 140:4186
TITLE: Identification of the Taste Enhancer Alapyridaine in Beef Broth and Evaluation of Its Sensory Impact by Taste Reconstitution Experiments
AUTHOR(S): Ottinger, Harald; Hofmann, Thomas
CORPORATE SOURCE: Deutsche Forschungsanstalt fuer Lebensmittelchemie, Garching, 85748, Germany
SOURCE: Journal of Agricultural and Food Chemistry (2003), 51(23), 6791-6796
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An essential compd. imparting the sweet taste to beef broth was investigated. Taste activity-guided fractionation of beef broth by ultrafiltration, gel permeation chromatog., and HPLC in combination with the recently developed comparative taste diln. anal. enabled the localization of a fraction possessing sweetness-enhancing activity upon degustation. Comparison of the chromatog., spectroscopic, and sensory data with those of the synthetic ref. compd. led to the identification of the sweetness-enhancing N-(1-carboxyethyl)-6-(hydroxymethyl)pyridinium-3-ol inner salt, named alapyridaine, which was recently isolated from heated aq. solns. of hexoses and L-alanine. After quantification of alapyridaine in beef broth, sensory anal. of synthetic beef taste recombinates spiked with synthetic alapyridaine in its "natural" concn. of 419 μg/L and comparison to the taste quality of a tastant recombinate lacking the alapyridaine revealed a significant increase in sweetness and umami character only when the alapyridaine was present in the recombinate. These data demonstrate for the 1st time that, in "natural" concns., the alapyridaine exhibited a pronounced effect on the overall taste quality of beef broth, in particular, on the sweet and umami character.

IT **501421-91-6**, Alapyridaine
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(identification of taste enhancer alapyridaine in beef broth and evaluation of its sensory impact by taste reconstitution expts.)

RN 501421-91-6 HCAPLUS
CN Pyridinium, 1-(1-carboxyethyl)-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

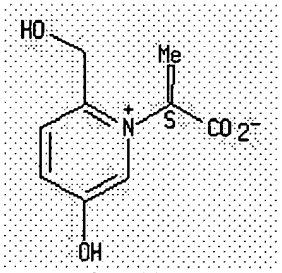
ACCESSION NUMBER: 2003:500969 HCAPLUS
DOCUMENT NUMBER: 139:337141
TITLE: (+)-(S)-Alapyridaine-A general taste enhancer?

AUTHOR(S): Soldo, Tomislav; Blank, Imre; Hofmann, Thomas
CORPORATE SOURCE: Deutsche Forschungsanstalt fuer Lebensmittelchemie, Garching, D-85748, Germany
SOURCE: Chemical Senses (2003), 28(5), 371-379
CODEN: CHSED8; ISSN: 0379-864X
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The threshold concns. for the sweet taste of glucose and sucrose, for the umami taste of monosodium l-glutamate (MSG) and guanosine-5'-monophosphate (GMP), as well as the salty taste of NaCl, were significantly decreased when alapyridaine was present. In contrast, perception of the bitter tastes of caffeine and L-phenylalanine, as well as of sour-tasting citric acid, was unaffected. Furthermore, alapyridaine was shown to intensify known taste synergisms such as, for example, the enhancing effect of L-arginine on the salty taste of NaCl, as well as that of GMP on the umami taste of MSG. The activity of (+)-(S)-alapyridaine could be obsd. not only in solns. of single taste compds., but also in more complex tastant mixts.; for example, the umami, sweet and salty taste of a soln. contg. MSG, sucrose, NaCl and caffeine was significantly modulated, thus indicating that alapyridaine is a general taste enhancer.

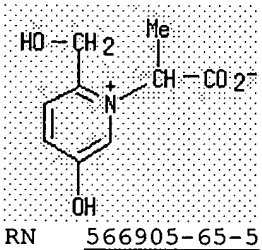
IT **501007-16-5**, (+)-(S)-Alapyridaine **501421-91-6** **566905-65-5**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(alapyridaine as general taste enhancer)

RN 501007-16-5 HCAPLUS
CN Pyridinium, 1-[(1S)-1-carboxyethyl]-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

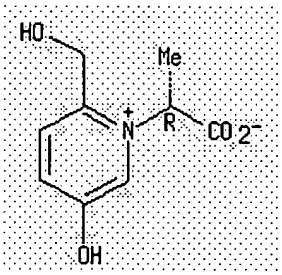


RN 501421-91-6 HCAPLUS
CN Pyridinium, 1-(1-carboxyethyl)-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)



RN 566905-65-5 HCAPLUS
CN Pyridinium, 1-[(1R)-1-carboxyethyl]-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

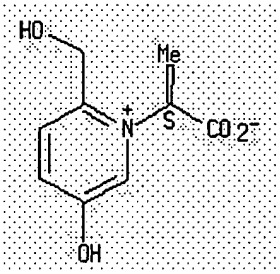
ACCESSION NUMBER: 2003:421335 HCAPLUS
DOCUMENT NUMBER: 139:133445
TITLE: Racemic and Enantiopure Synthesis and Physicochemical Characterization of the Novel Taste Enhancer N-(1-Carboxyethyl)-6-(hydroxymethyl)pyridinium-3-ol Inner Salt
AUTHOR(S): Villard, Renaud; Robert, Fabien; Blank, Imre; Bernardinelli, Gerald; Soldo, Tomislav; Hofmann, Thomas
CORPORATE SOURCE: Nestle Research Center, Lausanne, 1000, Switz.
SOURCE: Journal of Agricultural and Food Chemistry (2003), 51(14), 4040-4045
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:133445

AB Convenient syntheses were developed to obtain on a multigram scale the novel taste enhancer N-(1-carboxyethyl)-3-hydroxy-6-(hydroxymethyl)pyridinium (I), called alapyridaine, as a racemic mixt. and as pure (+)-(S) and (-)-(R) enantiomers, resp. 5-(Hydroxymethyl)-2-furaldehyde was used as key intermediate and was reacted with L-alanine under alk. conditions to obtain racemic I. Alternatively, reductive amination of 5-(hydroxymethyl)-2-furaldehyde with Raney-Ni/hydrogen and L- or D-alanine followed by mild oxidn. led to (+)-(S)-I and (-)-(R)-I, resp. Racemization was promoted under alk. and boiling conditions via a carbanion, the formation of which was facilitated by the electron-withdrawing effect of the iminium cation and the resonance-stabilizing capacity of the pyridinium moiety. Under these conditions, I was obtained in a 1:1 mixt. of the phenol I and phenolate (I-H) forms as shown by X-ray diffraction. Racemic I formed monoclinic crystals of high mol. organization in which the phenol-type (RS)-I, the phenolate-type (RS)-I-H, sodium cations, and ethanol mols. are present. The crystal structure of [Na(I)(I-H)?(C2H6O)] shows one-dimensional μ2-bridging-oxygen polymers stabilized by a three-dimensional network of ionic, hydrogen bond, and π-stacking interactions with channels occupied by solvent mols.

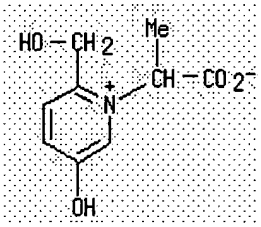
IT **501007-16-5P** **501421-91-6P** **566905-65-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of racemic and enantiopure N-(1-carboxyethyl)-3-hydroxy-6-(hydroxymethyl)pyridinium inner salt as novel taste enhancer)

RN 501007-16-5 HCAPLUS
CN Pyridinium, 1-[(1S)-1-carboxyethyl]-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

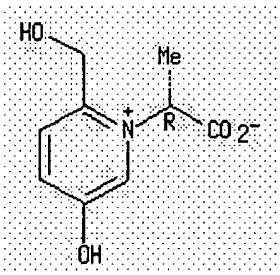


RN 501421-91-6 HCAPLUS
CN Pyridinium, 1-(1-carboxyethyl)-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)



RN 566905-65-5 HCAPLUS
CN Pyridinium, 1-[(1R)-1-carboxyethyl]-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

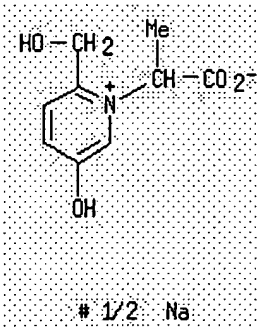
Absolute stereochemistry. Rotation (-).



IT **566905-67-7**
RL: PRP (Properties)
(prepn. of racemic and enantiopure N-(1-carboxyethyl)-3-hydroxy-6-(hydroxymethyl)pyridinium inner salt as novel taste enhancer and crystal structure)
RN 566905-67-7 HCAPLUS
CN Pyridinium, 1-(1-carboxyethyl)-5-hydroxy-2-(hydroxymethyl)-, inner salt, sodium salt, compd. with ethanol (4:2:1) (9CI) (CA INDEX NAME)

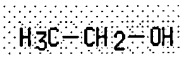
CM 1

CRN 566905-66-6
CMF C9 H11 N O4 . 1/2 Na



CM 2

CRN 64-17-5
CMF C2 H6 O



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:201514 HCAPLUS
DOCUMENT NUMBER: 138:221853
TITLE: Preparation of pyridinium-betaine compounds as taste enhancers
INVENTOR(S): Hofmann, Thomas; Ottinger, Harald; Frank, Oliver; Soldo, Tomislav; Blank, Imre; Villard, Renaud; Robert, Fabien
PATENT ASSIGNEE(S): Societe des Produits Nestle S.A., Switz.
SOURCE: Eur. Pat. Appl., 17 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

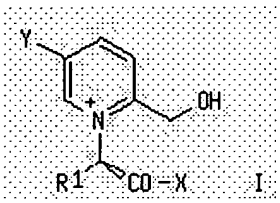
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1291342	A1	20030312	EP 2001-121349	20010906
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CA 2457950	AA	20030320	CA 2002-2457950	20020905
WO 2003022817	A1	20030320	WO 2002-EP10368	20020905
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1427703	A1	20040616	EP 2002-797989	20020905
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

JP 2005508902	T2	20050407	JP 2003-526893		20020905
US 2004171648	A1	20040902	US 2004-792369		20040302
PRIORITY APPLN. INFO.:			EP 2001-121349	A	20010906
			WO 2002-EP10368	W	20020905

OTHER SOURCE(S): MARPAT 138:221853

GI



I

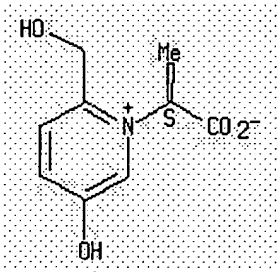
AB The invention concerns pyridinium-betaine compds. I (R1 is the side chain of a primary L-amino acid; X, Y are OH or O-), in which the counter ion is sodium, potassium, ammonium, calcium, magnesium, chloride, nitrate, carbonate, sulfate, phosphate, etc., for use as taste enhancers. Thus, treatment of 5-(hydroxymethyl)-2-furancarboxaldehyde with L-alanine in H2O/EtOH (1:1; pH 9.4) at reflux for 3 days afforded (S)-alapyridaine (I; R1 = Me, X = O-, Y = OH), which has a sweet taste.

IT **501007-16-5P 501007-17-6P 501007-18-7P**
501007-20-1P
RL: FFD (Food or feed use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyridinium-betaine compds. as taste enhancers)

RN 501007-16-5 HCAPLUS

CN Pyridinium, 1-[(1S)-1-carboxyethyl]-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

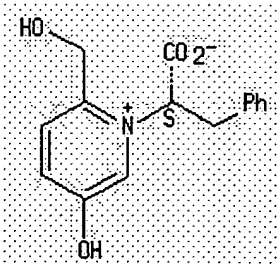
Absolute stereochemistry. Rotation (+).



RN 501007-17-6 HCAPLUS

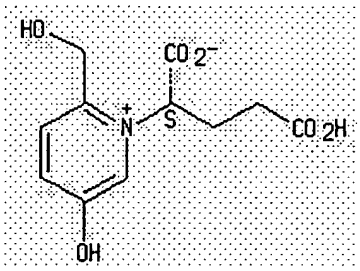
CN Pyridinium, 1-[(1S)-1-carboxy-2-phenylethyl]-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



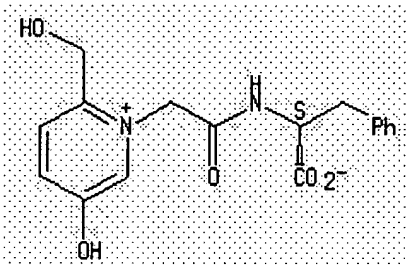
RN 501007-18-7 HCAPLUS
CN Pyridinium, 1-[(1S)-1,3-dicarboxypropyl]-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 501007-20-1 HCAPLUS
CN Pyridinium, 1-[2-[[(1S)-1-carboxy-2-phenylethyl]amino]-2-oxoethyl]-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:43135 HCAPLUS
DOCUMENT NUMBER: 138:237117
TITLE: Discovery and Structure Determination of a Novel Maillard-Derived Sweetness Enhancer by Application of the Comparative Taste Dilution Analysis (cTDA)
AUTHOR(S): Ottinger, Harald; Soldo, Tomislav; Hofmann, Thomas
CORPORATE SOURCE: Deutsche Forschungsanstalt fuer Lebensmittelchemie, Garching, D-85748, Germany
SOURCE: Journal of Agricultural and Food Chemistry (2003), 51(4), 1035-1041
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:237117

AB Application of a novel screening procedure, comparative taste diln. anal. (cTDA), on the non-solvent-extractable reaction products formed in a thermally processed aq. soln. of glucose and L-alanine led to the discovery of the presence of a sweetness-enhancing Maillard reaction product. Isolation, followed by LC-MS and 1D- and 2D-NMR measurements, and synthesis led to its unequivocal identification as I (alapyridaine; N-(1-carboxyethyl)-6-(hydroxymethyl)pyridinium-3-ol inner salt). I is itself tasteless but is the first nonvolatile, sweetness-enhancing Maillard reaction product to be reported. Depending on the pH value, the

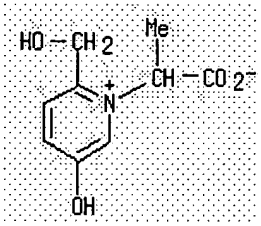
detection thresholds of sweet sugars, amino acids, and aspartame, resp., were found to be significantly decreased when I was present; for example, the threshold of glucose decreased by a factor of 16 in an equimolar mixt. of glucose and I. Studies on the influence of the stereochem. on taste-enhancing activity revealed that (+)-(S)-alapyridaine is the physiol. active enantiomer, whereas the (-)-(R)-enantiomer did not affect sweetness perception at all. Thermal processing of aq. solns. of I at 80? demonstrated a high thermal and hydrolytic stability of the sweetness enhancer; for example, more than 90 or 80% of I was recovered when heated for 5 h at pH 7.0, 5.0, or 3.0, resp.

IT **501421-91-6P**

RL: ANT (Analyte); BSU (Biological study, unclassified); FFD (Food or feed use); FMU (Formation, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); USES (Uses)
(alapyridaine Maillard-type sweetness enhancer)

RN 501421-91-6 HCAPLUS

CN Pyridinium, 1-(1-carboxyethyl)-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)



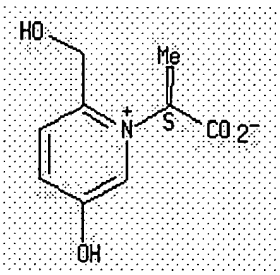
IT **501007-16-5**

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(alapyridaine Maillard-type sweetness enhancer)

RN 501007-16-5 HCAPLUS

CN Pyridinium, 1-[(1S)-1-carboxyethyl]-5-hydroxy-2-(hydroxymethyl)-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	53.58	222.05

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.75	-6.75

FILE 'CAOLD' ENTERED AT 13:56:18 ON 10 MAY 2006

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

Cl
N
CH2
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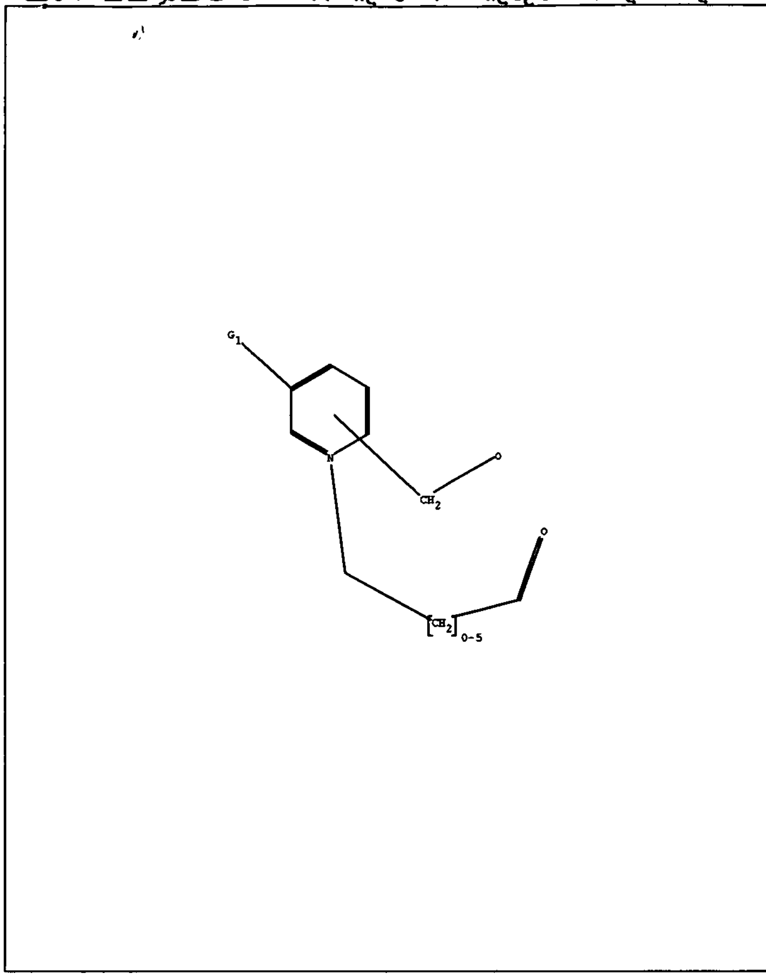

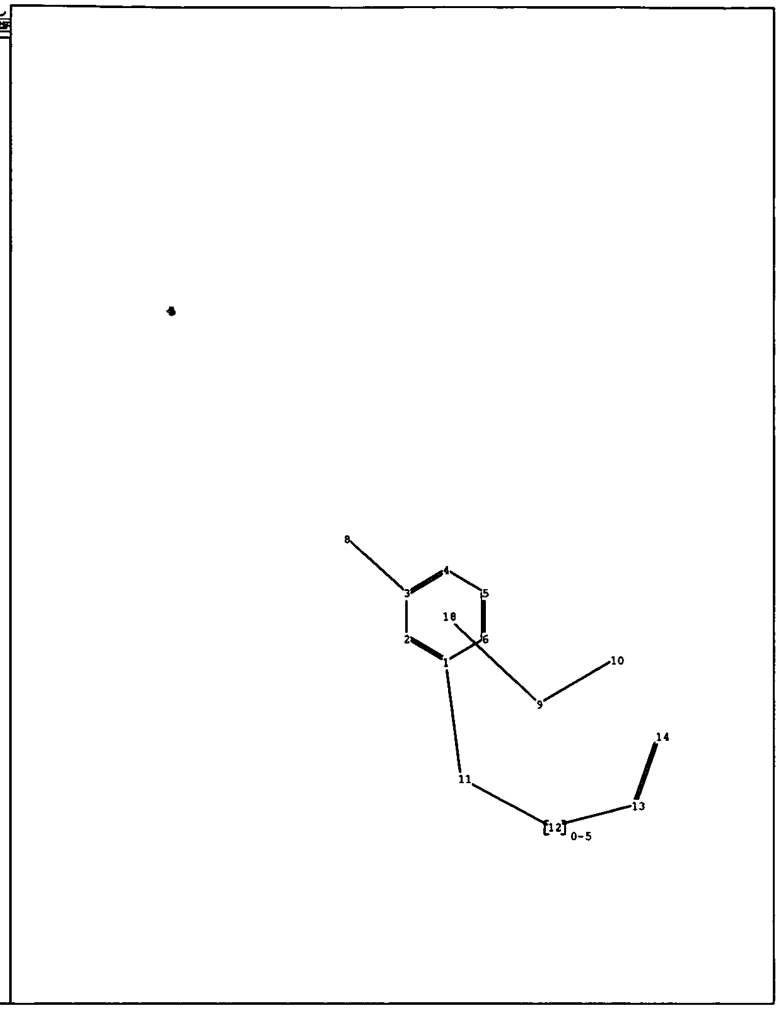

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ring nodes :
1 2 3 4 5 6
chain bonds :
1-11 3-8 9-10 11-12 12-13 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-11 3-8 13-14
exact bonds :
9-10 11-12 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS
9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS
18:CLASS

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=> d his

     (FILE 'HOME' ENTERED AT 13:51:50 ON 10 MAY 2006)

     FILE 'REGISTRY' ENTERED AT 13:52:13 ON 10 MAY 2006
L1             STRUCTURE UPLOADED
L2           1 S L1
L3          17 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 13:54:19 ON 10 MAY 2006
L4           9 S L3
L5           9 S L4 AND HOFMANN, T?/AU

     FILE 'CAOLD' ENTERED AT 13:56:18 ON 10 MAY 2006

=> s l3
L6           0 L3

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.44     222.49

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -6.75

FILE 'REGISTRY' ENTERED AT 13:57:09 ON 10 MAY 2006
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:    9 MAY 2006  HIGHEST RN 883631-57-0
DICTIONARY FILE UPDATES:   9 MAY 2006  HIGHEST RN 883631-57-0

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*********************************************************************
*                                                                   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                   *
*********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
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on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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Uploading structure

L7 STRUCTURE UPLOADED

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L7 HAS NO ANSWERS
L7 STR

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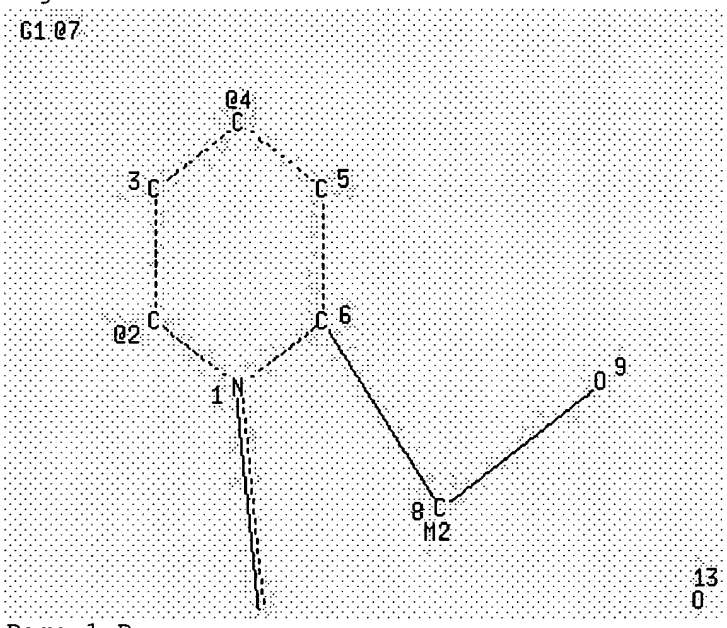

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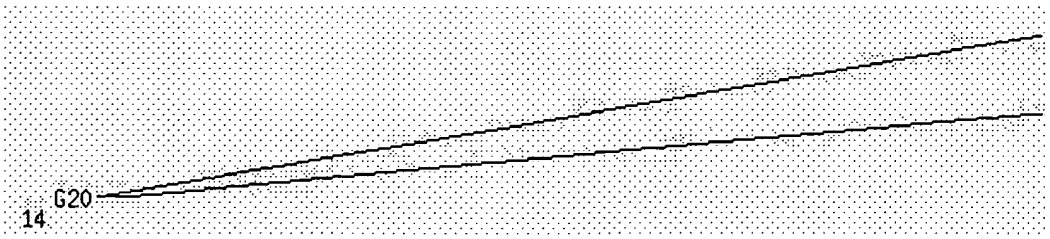

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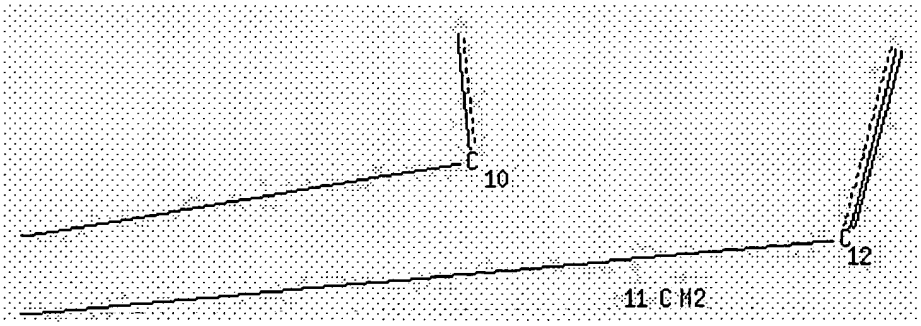

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VPA 7-2/4 S
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NSPEC    IS R       AT   5
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NSPEC    IS C       AT   9
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NSPEC    IS C       AT  11
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  16

STEREO ATTRIBUTES: NONE


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SAMPLE SCREEN SEARCH COMPLETED -      170 TO ITERATE

100.0% PROCESSED      170 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         2618 TO     4182
PROJECTED ANSWERS:               0 TO        0

L8            0 SEA SSS SAM L7

=> s l7 full
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DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
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100.0% PROCESSED     3277 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L9            0 SEA SSS FUL L7

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Uploading structure

L10     STRUCTURE UPLOADED

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L10 HAS NO ANSWERS
L10             STR
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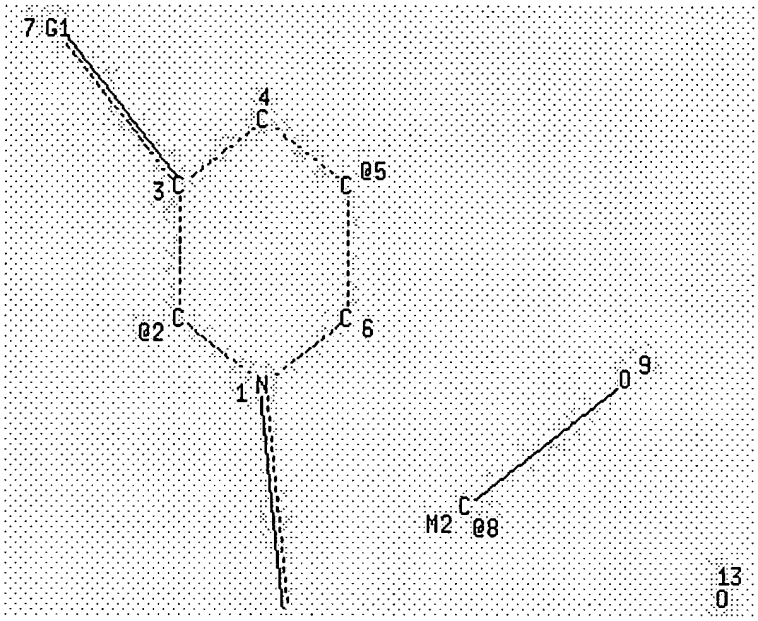
O 15 S 16

Page 1-A



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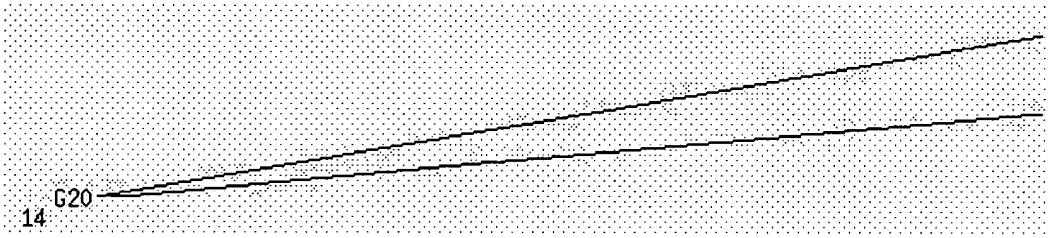
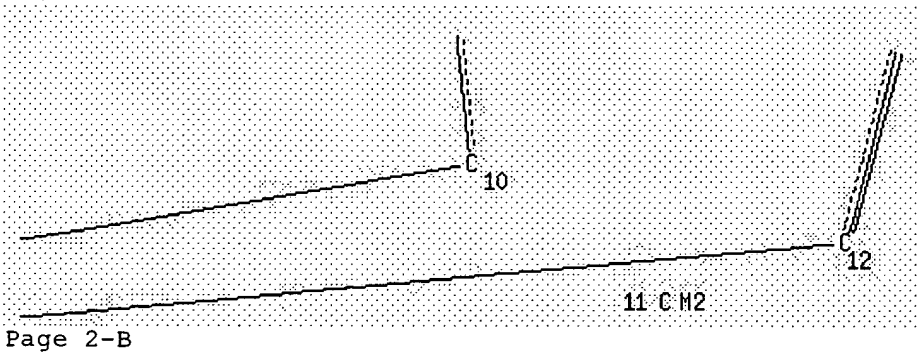


Page 2-A



Page 2-B

VAR G1=15/16
REP G20=(0-5) 11-10 11-12
VPA 8-2/5 S
NODE ATTRIBUTES:
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HCOUNT IS M2 AT 11
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
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NSPEC IS C AT 7
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DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   8  9 10 11 12 13 15 16
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  16

STEREO ATTRIBUTES: NONE


=> s l10
SAMPLE SEARCH INITIATED 13:59:51 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      137 TO ITERATE

100.0% PROCESSED      137 ITERATIONS                              2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         2038 TO     3442
PROJECTED ANSWERS:               2 TO      124

L11           2 SEA SSS SAM L10

=> s l10 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 166.50 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 13:59:56 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     2571 TO ITERATE

100.0% PROCESSED     2571 ITERATIONS                             21 ANSWERS
SEARCH TIME: 00.00.01

L12          21 SEA SSS FUL L10

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             335.20     557.69

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                 ENTRY    SESSION
CA SUBSCRIBER PRICE                               0.00      -6.75

FILE 'HCAPLUS' ENTERED AT 13:59:59 ON 10 MAY 2006
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FILE COVERS 1907 - 10 May 2006 VOL 144 ISS 20
FILE LAST UPDATED: 9 May 2006 (20060509/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L13          28 L12

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             54 HOFMAN, T?/AU
L14           0 L13 AND HOFMAN, T?/AU

=> s l13 and ottinger, h?/au
            103 OTTINGER, H?/AU
L15           0 L13 AND OTTINGER, H?/AU

=> s l13 and frank, o?/au
            232 FRANK, O?/AU
L16           0 L13 AND FRANK, O?/AU

=> s l13 and soldo, t?/au
             14 SOLDO, T?/AU
L17           0 L13 AND SOLDO, T?/AU

=> s l13 and blank, i?/au
            193 BLANK, I?/AU
L18           0 L13 AND BLANK, I?/AU

=> s l13 and villard, r?/au
             17 VILLARD, R?/AU
L19           0 L13 AND VILLARD, R?/AU

=> s l13 and robert, f?/au
            481 ROBERT, F?/AU
L20           0 L13 AND ROBERT, F?/AU

=> d l13, ibib abs hitstr, 1-28

L13  ANSWER 1 OF 28  HCAPLUS  COPYRIGHT 2006 ACS on STN
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Full Text | Cited References

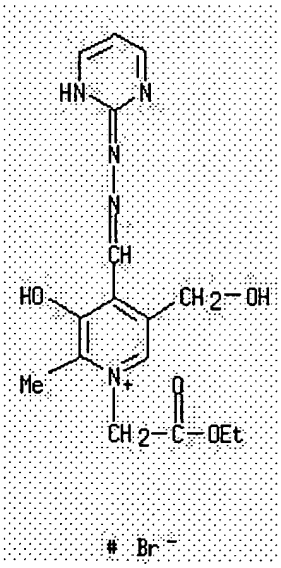
ACCESSION NUMBER: 2005:240979 HCAPLUS
DOCUMENT NUMBER: 144:69699
TITLE: Growth inhibition of drug-resistant species of Plasmodium falciparum by domain structured N1,N2-derivatized hydrazines: denticity effects, redox switches, and reductant-driven redox-cycling
AUTHOR(S): Sarel, S.; Iheanacho, E. N.; Avramovici-Grisaru, S.
CORPORATE SOURCE: Department of Medicinal Chemistry, The Hebrew University of Jerusalem, Jerusalem, 91120, Israel
SOURCE: Medicinal Chemistry (2005), 1(2), 159-171
CODEN: MCEHAJ; ISSN: 1573-4064

PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Six analogs of bidentate 1-[pyridoxylidene]-2-phenylhydrazine, twelve analogs of N2O-tridentate 1-[pyridoxylidene]-2-[heteroaryl]hydrazine, and four O2N-tridentate analogs of 1-[pyridoxylidene]-2-[heteroaroyl] hydrazines were synthesized and characterized. Their solns. in water and DMSO were assayed in vitro for activity against a chloroquine-resistant species of P. falciparum. The O2N-tridentate group was essentially inactive, whereas the bidentate group, with N and O ligating atoms, exhibited slight activity against late-stage trophozoites and schizonts of P. falciparum. The N2O-tridentate group, by contrast, was remarkably active against resistant P. falciparum, highlighting the importance of the Denticity Effect in this system. It was assumed that the pyridoxal-based chelator acted as an iron redox mediator, controlling the first coordination sphere and, therefore, the immediate chem. environment of the iron. Chelation of iron-(II) presumably facilitates its oxidn. The Fe(II) ? Fe(III) intra-electron transfer, may be viewed as a switch ("redox switch"), controlling the thermodn. stability and kinetic lability of the coordination shell. The redox-switch is accompanied by the appearance of a carbon-based Fe-(III)-chelate radical, capable of donating its free electron to the parasite-DNA, thus causing death. The antimalarial N2O-tridentate Fe(III)-chelates appear to be prone to redox-switch, and tend to be converted into their Fe(II) species, whereas the inactive O2N-tridentate analogs apparently cannot do so.

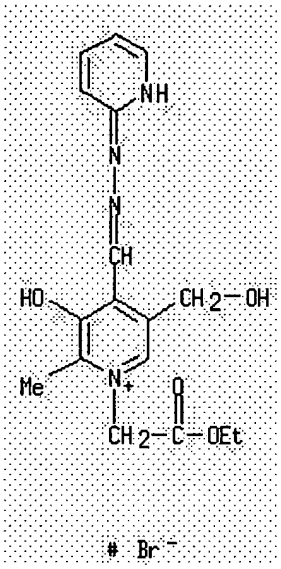
IT **124050-83-5**
RL: PAC (Pharmacological activity); BIOL (Biological study)
(prepn., antimalarial activity, and growth inhibition of drug resistant plasmodium falciparum of pyridoxal hydrazine chelators using condensation of pyridoxal as the key step)

RN 124050-83-5 HCAPLUS
CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyrimidinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



IT **124076-31-9**
RL: PAC (Pharmacological activity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(prepn., antimalarial activity, and growth inhibition of drug resistant plasmodium falciparum of pyridoxal hydrazine chelators using condensation of pyridoxal as the key step)

RN 124076-31-9 HCAPLUS
CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyridinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:774487 HCAPLUS
DOCUMENT NUMBER: 134:336127
TITLE: Chelator-induced iron excretion in iron-overloaded marmosets
AUTHOR(S): Sergejew, Thomas; Forgiarini, Peter; Schnebli, Hans-Peter
CORPORATE SOURCE: Novartis Pharma AG, Basel, CH-4002, Switz.
SOURCE: British Journal of Haematology (2000), 110(4), 985-992
CODEN: BJHEAL; ISSN: 0007-1048
PUBLISHER: Blackwell Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To test new orally active Fe chelators in a predictive way, a primate model was developed. This model makes use of the marmoset monkey (Callithrix jacchus) and its overall design is similar to a previously reported monkey model. However, this new model enables a higher compd. throughput and requires lower amts. of test compd. because the animals are much easier to handle and have much lower body wts. The marmosets were Fe-overloaded by 3 i.p. injections of Fe (III) hydroxide polyisomaltose. For the Fe-balance studies, the animals were kept in metabolic cages and were maintained on a low-Fe diet to reduce fecal background. After compd. administration, the excretion of Fe in urine and feces was followed for 2 d. A series of well-known chelators was tested for validation of the model. In particular, comparison of the Fe-clearing properties of DFO, L1, CP94, and HBED in marmosets and humans demonstrated the predictive value of the model and justify the authors' expectation that if Fe chelators such as CGP65015, ICL670A, and CGP75254A are active in marmosets, they will be active in humans as well.

IT 156550-29-7, CGP 43902B
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Ychelator-induced Fe excretion in Fe-overloaded marmosets)

RN 156550-29-7 HCAPLUS
CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyrimidinylhydrazono)methyl]-, methanesulfonate (salt) (9CI) (CA INDEX NAME)

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CRN 156550-28-6
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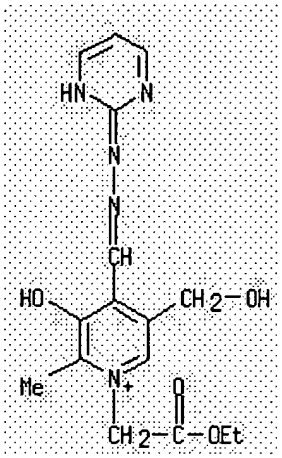

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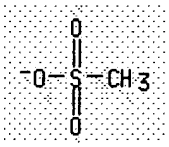


REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Cited References

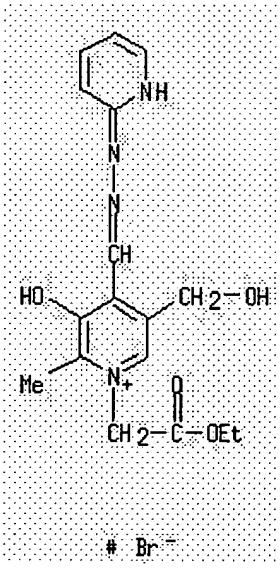
ACCESSION NUMBER: 2000:434893 HCAPLUS
DOCUMENT NUMBER: 133:232525
TITLE: Inhibition of in vitro lymphoproliferation by three novel iron chelators of the pyridoxal and salicyl aldehyde hydrazone classes
AUTHOR(S): van Reyk, D.; Sarel, S.; Hunt, N.
CORPORATE SOURCE: Department of Pathology, University of Sydney, 2006, Australia
SOURCE: Biochemical Pharmacology (2000), 60(4), 581-587
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The capacity of three novel iron chelators, namely 1-[N-ethoxycarbonylmethylpyridoxylidenium]-2-[2'-pyridyl]hydrazine bromide (EPH), 1-[5'-bromosalicylidene]-2-[2''-pyridyl]hydrazine (BsPH), and 1-pyridoxylidene-2-[1'-phthalazyl]hydrazine dihydrochloride (PPhH), to inhibit the proliferation of mitogen-stimulated murine lymph node cells was examd. in vitro. All three are of the aryl hydrazone class, the prototype of which is pyridoxal isonicotinoyl hydrazone. The chelators inhibited lymphoproliferation at low micromolar concns. EPH and PPhH had an inhibitory capacity comparable to that of desferrioxamine (ic50: 3 and 2 μM, resp.), whereas BsPH was more potent (ic50 < 1 μM). The inhibitory effects of the chelator were not due to cell cytotoxicity and could be abrogated by pretreating the chelator with iron. Time-course studies established a site of action for the chelators at the G1/S phase transition. These agents warrant further investigation for their potential as immunosuppressants.

IT **124076-31-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(inhibition of in vitro lymphoproliferation by three novel iron chelators of the pyridoxal and salicyl aldehyde hydrazone classes)

RN 124076-31-9 HCAPLUS

CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyridinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:464048 HCAPLUS
DOCUMENT NUMBER: 131:82989
TITLE: Nitric oxide-releasing chelating agents and their therapeutic use
INVENTOR(S): Towart, Robertson; Karlsson, Jan Olof Gustav; Wistrand, Lars Goran; Malmgren, Hakan
PATENT ASSIGNEE(S): Nycomed Imaging A/S, Norway
SOURCE: PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9933823	A1	19990708	WO 1998-GB3840		19981218
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA					
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
AU 9917702	A1	19990719	AU 1999-17702		19981218
EP 1060174	A1	20001220	EP 1998-962567		19981218
EP 1060174	B1	20040922			
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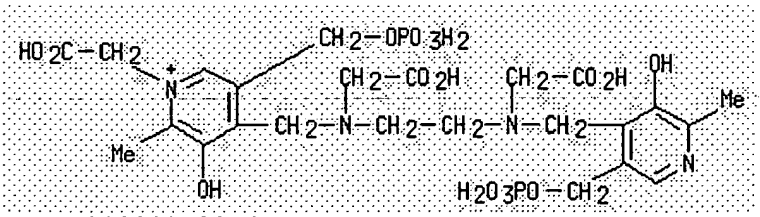
JP 2001527072	T2	20011225	JP 2000-526505		19981218
AT 277038	E	20041015	AT 1998-962567		19981218
ZA 9811825	A	19990708	ZA 1998-11825		19981223
US 6391895	B1	20020521	US 2000-599862		20000623
PRIORITY APPLN. INFO.:			GB 1997-27226	A	19971223
			US 1998-76793P	P	19980304
			GB 1998-5450	A	19980313
			WO 1998-GB3840	W	19981218

OTHER SOURCE(S): MARPAT 131:82989

AB Chelating agents, in particular dipyridoxyl and aminopolycarboxylic acid-based chelating agents, and their metal chelates, when linked directly or indirectly to at least one nitric oxide-releasing moiety, or when use in combination with nitric oxide or a nitric oxide-releasing moiety, have been found to be effective in treating a variety of disorders. In particular, such compds. may be used in treating conditions assocd. with the presence of free radicals in the body, e.g. reperfusion injuries, and in reducing the cardiotoxicity of anti-tumor agents, e.g. anthracyclines and/or paclitaxel.

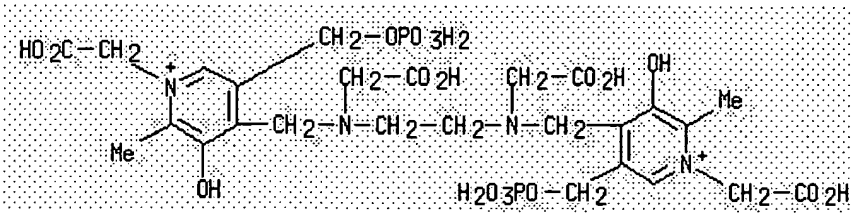
IT **230302-21-3D**, conjugates with nitric oxide-releasing moieties
230302-22-4D, conjugates with nitric oxide-releasing moieties
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(nitric oxide-releasing chelating agents, and therapeutic use)

RN 230302-21-3 HCAPLUS
CN Pyridinium, 1-(carboxymethyl)-4-[[(carboxymethyl)[2-[(carboxymethyl)[[3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]-4-pyridinyl]methyl]amino]ethyl]amino]methyl]-3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]- (9CI) (CA INDEX NAME)



RN 230302-22-4 HCAPLUS
CN Pyridinium, 4,4'-[1,2-ethanediylbis[[(carboxymethyl)imino]methylene]]bis[1-

(carboxymethyl)-3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]- (9CI) (CA INDEX NAME)

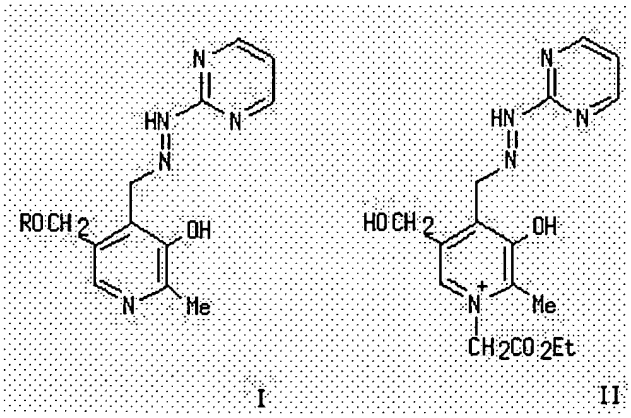


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 5 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1999:32713 HCAPLUS
DOCUMENT NUMBER: 130:182292
TITLE: Iron chelators of the pyridoxal-based class. Part 7. The synthesis and single crystal structure of 1-(N-ethoxycarbonylmethylpyridoxyledenium)-2-(pyrimidyl)hydrazine salts
AUTHOR(S): Sarel, Shalom; Avramovici-Grisaru, Shelly; Cohen, Shmuel
CORPORATE SOURCE: Department of Medicinal Chemistry, Hebrew University of Jerusalem, Jerusalem, 91904, Israel
SOURCE: Heterocycles (1998), 49, 393-404
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I II

AB The syntheses of 1-pyridoxylidene-2-(2'-pyrimidyl)hydrazine (I; R = H), 1-(N-methylpyridoxylidenium)-2-(2'-pyrimidyl)hydrazine iodide (I; R = Ac), and 1-(N-ethoxycarbonylmethylpyridoxylidenium)-2-(pyrimidyl)hydrazine bromide (II?Br-), and 1-(N-ethoxycarbonylmethylpyridoxylidenium)-2-(2'-pyrimidyl)hydrazine perchlorate (II?ClO4-) are described. The single-crystal structure of II?ClO4- was detd. from three-dimensional x-ray data. Compd. II?ClO4-, C16H22N5O8Cl crystallizes in the space group P21/c with Z = 4 and the following cell dimensions: a = 12.363 (3) Å, b = 17.168(5) Å, c = 9.657(3) Å. The x-ray data confirm that II?ClO4- crystallizes in the di-polar form, as a planar 20-membered ring dimer. All the three proton-donors

(O1-H, O2-H, and N3-H), and only three (N2, N5, O2) of the five available proton-acceptors II?ClO4-, are utilized in hydrogen-bonding.

IT **220680-33-1P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis and single crystal structure of 1-(N-ethoxycarbonylmethylpyridoxylidenium)-2-(2-pyrimidinyl)hydrazine salts)

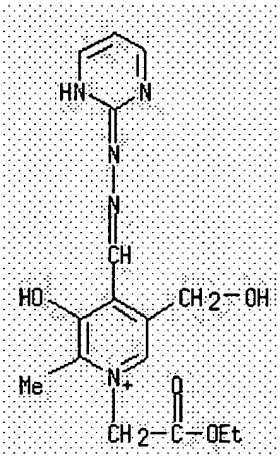
RN 220680-33-1 HCAPLUS

CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyrimidinylhydrazono)methyl]-, perchlorate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 156550-28-6

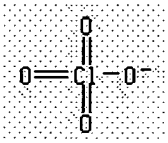
CMF C16 H20 N5 O4



CM 2

CRN 14797-73-0

CMF Cl O4



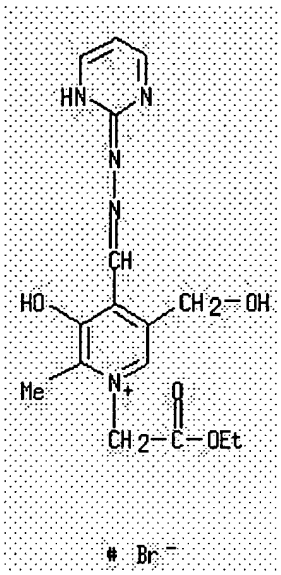
IT **124050-83-5P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and single crystal structure of 1-(N-ethoxycarbonylmethylpyridoxylidenium)-2-(2-pyrimidinyl)hydrazine salts)

RN 124050-83-5 HCAPLUS

CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyrimidinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 6 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

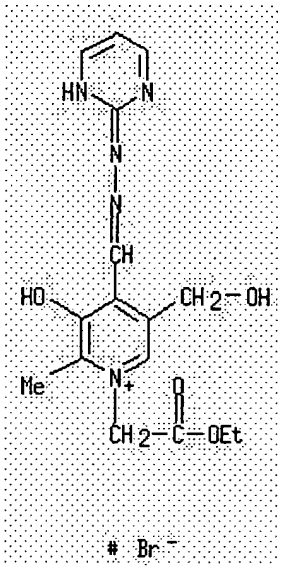
ACCESSION NUMBER: 1999:23873 HCAPLUS
DOCUMENT NUMBER: 130:182286
TITLE: Domain-Structured N1,N2-Derivatized Hydrazines as Inhibitors of Ribonucleoside Diphosphate Reductase: Redox-Cycling Considerations
AUTHOR(S): Sarel, Shalom; Fizames, C.; Lavelle, Francois; Avramovici-Grisaru, Shelly
CORPORATE SOURCE: Department of Medicinal Chemistry, Hebrew University of Jerusalem, Jerusalem, 91120, Israel
SOURCE: Journal of Medicinal Chemistry (1999), 42(2), 242-248
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Eight analogs of 1-[5-halosalicylidene]-2-[2-pyridinoyl]hydrazine and -[2-pyridyl]hydrazine, four of 1-[pyridoxylidene]-2-[2-pyridinoyl]hydrazine, seven of 1-[pyridoxylidene]-2-[2-pyridyl]hydrazine, and one each of 1,2-bis[pyridoxylidene]diaminoethane and bis[pyridoxylidenehydrazino]phthalazine were synthesized. Their solns. in DMF were assayed for activity against the metalloenzyme ribonucleoside diphosphate reductase (RdR), prepd. from a s.c. growing murine tumor (sarcoma 180) implanted in B6D2F3 male mice. The 14C-labeled CDP reductase was assayed by the modified method of Takeda and Weber, in which [14C]cytidine was sepd. from deoxycytidine by thin-layer chromatog. on cellulose foil. Distribution of radioactivity was assessed with an automatic TLC linear analyzer. Of the 31 compds. tested, 13 were essentially inactive, 7 were highly active against RdR, and the remaining 20 were slightly more active than hydroxyurea (used as a ref. compd.). The mechanism of inhibition is discussed in terms of three alternative pathways, initiated by sequestration of iron embedded in the R1 subunit of the metalloenzyme to form a C-centered chelate radical (via redox cycling). Alternatively, the latter could either reduce the tyrosyl radical or intercept radicals generated in the redn. process.

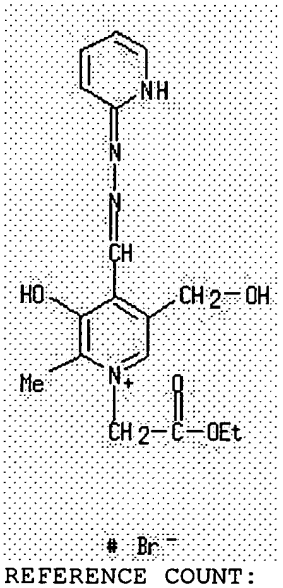
IT **124050-83-5** **124076-31-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); BIOL (Biological study)
(prepn. and ribonucleoside diphosphate reductase inhibiting activity of pyridinoyl- and pyridylhydrazines)

RN 124050-83-5 HCAPLUS
CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyrimidinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



RN 124076-31-9 HCAPLUS
CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyridinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 7 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

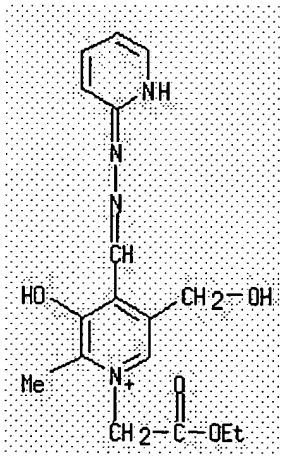
Full Text | Citing References

ACCESSION NUMBER: 1995:372624 HCAPLUS
DOCUMENT NUMBER: 122:177689
TITLE: Iron chelators of the pyridoxal 2-pyridyl hydrazone class. Part 4. pKa values of the chelators and their

relevance to biological properties
AUTHOR(S): Doungdee, Prayong; Sarel, Shalom; Wongvisetsirikul, Nipon; Avramovici-Grisaru, Shelly
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Hebrew Univ. Sch. of Pharmacy, Jerusalem, 91120, Israel
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1995), (2), 319-23
CODEN: JCPKBH; ISSN: 0300-9580
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The proton binding consts. (pKa) and species distribution over pH range 1.5-12.0 of two types of biol. active iron chelators: (a) pyridoxal type (Lx) - pyridoxal 2-pyridyl hydrazone (PPH) and pyridoxal isonicotinoyl hydrazone (PIH); (b) pyridoxal-betaine type (Ly) - 1-[N-methyl-pyridoxylidenium]-2-[2'-pyridyl]hydrazine iodide (MPH) and 1-[N-ethoxy-carbonylmethylpyridoxylidenium]-2-[2'-pyridyl]hydrazine bromide (EPH) have been detd. by glass electrode potentiometry. The lowest pK value in type (a), in the range 2.62 (PPH)-2.45 (PIH) was assigned to pyridinium protonation; the following ionization consts., pKa2 = 4.63 (PPH)-4.54 (PIH), to pyridoxylidenium protonation; pKa3 = 7.96 (PPH)-7.44 (PIH), to phenolate protonation, and pKa4 = 9.96 (PIH)-9.84 (PPH) to amine-hydrazone protonation. At pH <2, all ligands exist in the resp. protonated forms (H4Lx2+, H3Ly2+ and H3Lx+) and at pH >11, in the fully deprotonated forms (Lx2+, and Ly-). At pH ~ 5.0, the pyridoxal-betaines, MPH and EPH, exist predominantly as zwitterions, whereas PPH and PIH are present at that pH predominantly in the neutral, non-zwitterionic, H2Lx form. At higher pH (7.2), PPH and PIH, are present as mixts. of the neutral and the neg. charged monodeprotonated forms.

IT **161535-45-1**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(structure effect on ionization consts. of iron chelators)
RN 161535-45-1 HCAPLUS
CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyridinylhydrazono)methyl]- (9CI) (CA INDEX NAME)



L13 ANSWER 8 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1995:332266 HCAPLUS
DOCUMENT NUMBER: 122:186677
TITLE: Iron chelators of the pyridoxal 2-pyridyl hydrazone

class. Part III. Ionization and conformational characteristics of the ligands

AUTHOR(S): Doungdee, Prayong; Sarel, Shalom; Ringel, Israel; Gibson, Dan; Wongvisetsirikul, Nipon; Avramovici-Grisaru, Shelly

CORPORATE SOURCE: Dep. Pharm. Chem., Hebrew Univ. Sch. Pharm., Jerusalem, 91120, Israel

SOURCE: Heterocycles (1995), 40(1), 241-8
CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

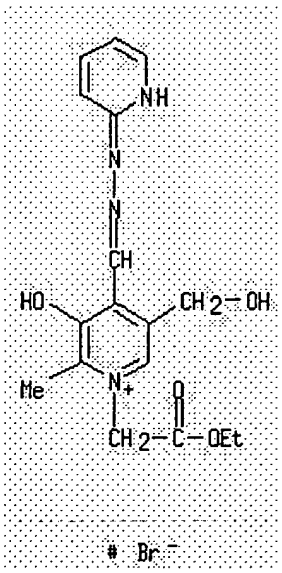
AB PKa values of three biol. active iron chelators: pyridoxal 2-pyridyl hydrazone (PPH), 1-[N-methylpyridoxylidenium]-2-[2'-pyridyl]hydrazine iodide (MPH), 1-[N-ethoxycarbonylmethylpyridoxylidenium]-2-[2'-pyridyl]hydrazine bromide (EPH) have been detd. by a combination of ab initio calcns. and pH-dependence of 13C NMR spectroscopy. In conformity with pyridoxal isonicotinoyl hydrazone (PIH), all ligands included in this study the pKa values invariably increase in the ordering: pyridinium protonation < pyridoxylidenium protonation < phenolate protonation < amine-hydrazone protonation < alkoxide protonation. Identical ordering was obtained by ab initio calcns., based on STO-3G set. Mulliken population anal. indicates that the conformer of the lowest energy of PPH, (I), contains an internal 6-membered-ring H-bond. Rotation about C3-C8 bond in (I), to yield conformer (IV), requires 8.8 kcal/mol, whereas its internal H-bonding. (I ? II) accounts for 5.8 kcal/mol. Protonation of (I) lowers significantly energies both of I ? V (6.5 kcal), and I ? VI (2.5 kcal) transitions.

IT **124076-31-9**

RL: PRP (Properties)
(ionization and conformational characteristics of pyridoxal 2-pyridyl hydrazone class ligand iron chelators)

RN 124076-31-9 HCAPLUS

CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyridinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



L13 ANSWER 9 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1994:473807 HCAPLUS
DOCUMENT NUMBER: 121:73807
TITLE: The action of nine chelators on iron-dependent radical damage
AUTHOR(S): Dean, Roger T.; Nicholson, Philip
CORPORATE SOURCE: Cell Biol. Group, Heart Res. Inst., Camperdown/Sydney, 2050, Australia
SOURCE: Free Radical Research (1994), 20(2), 83-101
CODEN: FRARER; ISSN: 1071-5762
DOCUMENT TYPE: Journal
LANGUAGE: English

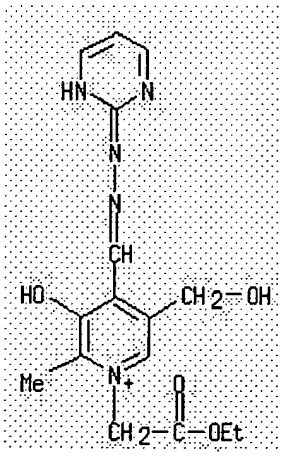
AB Nine iron chelators were tested in 5 systems for their effects on radical generation and conversion at chelator:iron molar ratios of 0.1-10. Stimulation of radical generation might distinguish toxic from safer chelators. Radical-generating reactions which represent different aspects of iron (ferrous and ferric) availability were studied: (a) the reaction with H2O2 to hydroxylate benzoate; (b) the oxidn. of ascorbate; (c) the reaction with H2O2 to fragment proteins; (d) the reaction with H2O2 to permit amplified chemiluminescence; and (e) the induction of peroxidn. of mitochondrial membrane lipids. The compds. used were HBED, CP130, Desferal, EDTA, pyridine hydrazone (CGP 43'902B), Ferrozine, CP 94 (CGP 46'700), L1 (CGP 37 391) and rhodotorulic acid (CGP 45 274). Only the hexadentate compds. HBED, CP130 and Desferal were uniformly inhibitory ("protective"). The protective compds. were also apparently more stable during radical fluxes than the other chelators.

IT **156550-29-7**, CGP 43902B
RL: BIOL (Biological study)
(radical reactions inhibition by, as iron chelator)

RN 156550-29-7 HCAPLUS
CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyrimidinylhydrazono)methyl]-, methanesulfonate (salt) (9CI) (CA INDEX NAME)

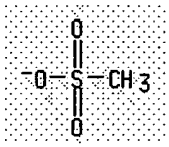
CM 1

CRN 156550-28-6
CMF C16 H20 N5 O4



CM 2

CRN 16053-58-0
CMF C H3 O3 S



L13 ANSWER 10 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

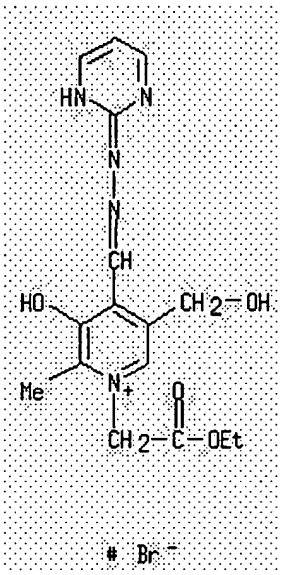
Full Text | Other References

ACCESSION NUMBER: 1992:524178 HCAPLUS
DOCUMENT NUMBER: 117:124178
TITLE: In vitro effects of three iron chelators on mitogen-activated lymphocytes: identification of differences in their mechanisms of action
AUTHOR(S): Van Reyk, D. M.; Sarel, S.; Hunt, N. H.
CORPORATE SOURCE: Dep. Pathol., Univ. Sydney, Australia
SOURCE: International Journal of Immunopharmacology (1992), 14(5), 925-32
CODEN: IJIMDS; ISSN: 0192-0561
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effects of three iron chelators (ADR-529/ICF-187; omadine/pyrithione; and a newly synthesized pyridoxal-based iron chelator,SAG-15) on cultured BALB/c murine lymph node cell stimulated with phorbol myristate acetate and ionomycin have been investigated. All three agents were found to inhibit [3H]-thymidine incorporation after 66-72 h incubation. Pretreatment of ADR-529 and omadine with Fe(III) or Fe(II) ions did not prevent their inhibitory effects. However, pretreatment of SAG-15 with Fe(II) or Fe(III) ions led to a significant increase in the ID50. Time-course studies of cell viability and thymidine incorporation demonstrated that the inhibitory effect of omadine was attributable to cell killing while for ADR-529 and SAG-15 there were both cytostatic and cytotoxic effects. Cell cycle anal. showed that treatment of cells with ADR-529 led to arrest in G2/M while treatment with SAG-15 led to a G0/G1 arrest. Iron has an obligatory role in T-lymphocyte activation that may be related to the formation of reactive oxygen species. SAG-15 is a new iron chelator that will help in the elucidation of the precise role of iron in lymphoproliferation. Since SAG-15 is an extremely effective iron chelator in vivo it has potential as an immunosuppressive agent.

IT **124050-83-5**, SAG 15
RL: BIOL (Biological study)
(T-lymphocyte proliferation inhibition by, as iron chelator)

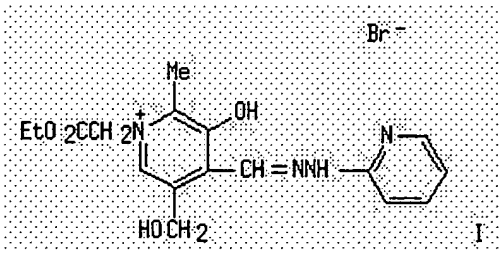
RN 124050-83-5 HCAPLUS
CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyrimidinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



L13 ANSWER 11 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1991:622835 HCAPLUS
DOCUMENT NUMBER: 115:222835
TITLE: Growth inhibition of Plasmodium falciparum involving carbon centered iron-chelate radical (L.ovrhdot., X-)-iron(III) based on pyridoxal-betaine. A novel type of antimalarials active against chloroquine-resistant parasites
AUTHOR(S): Iheanacho, Eugene N.; Sarel, Shalom; Samuni, Amram; Avramovici-Grisaru, Schelly; Spira, Dan T.
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Free Radical Research Communications (1991), 15(1), 1-10
CODEN: FRRCEX; ISSN: 8755-0199
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



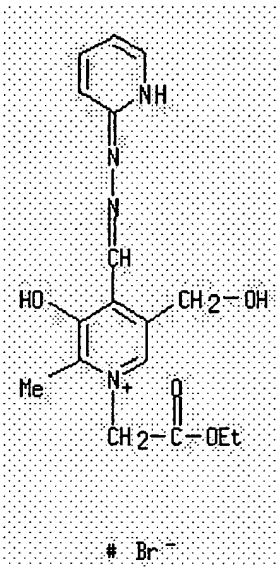
AB Malaria parasites have been shown to more susceptible to oxidative stress than their host erythrocytes. In the present work, a chloroquine resistant malaria parasite, P. falciparum (FCR-3) was found to be susceptible in vitro to the pyridoxal-based iron chelator L2-9 (I); 2 h exposure to 20 μM L2-9 was sufficient to irreversibly inhibit parasite growth. Desferrioxamine blocked the drug effect, indicating the requirement for iron. Oxygen however, was not essential. Spectrophotometric anal. showed that under anoxic conditions, L2-9-Fe(II) chelate undergoes an intramol. redox reaction which presumably involves a one-electron transfer and is expected to result in the formation of free

radical. Spin trapping coupled to ESR studies of L2-9-iron chelate showed that L2-9-Fe(II) produced free radicals both in the presence and absence of cells, while L2-9-Fe(III) produced free radicals only in the presence of actively metabolizing cells.

IT **124076-31-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antimalarial activity of, iron sequestering and free radical generation by)

RN 124076-31-9 HCAPLUS

CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyridinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



L13 ANSWER 12 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1991:484691 HCAPLUS
DOCUMENT NUMBER: 115:84691
TITLE: A comparative evaluation of iron clearance models
AUTHOR(S): Bergeron, Raymond J.; Streiff, Richard R.; Wiegand, Jan; Vinson, J. R. Timothy; Luchetta, Gabriel; Evans, Kimberly M.; Peter, Heinrich; Jenny, Hans Beat
CORPORATE SOURCE: Dep. Med. Chem., Univ. Florida, Gainesville, FL, 32610, USA
SOURCE: Annals of the New York Academy of Sciences (1990), 612(Cooley's Anemia Symp., 6th, 1990), 378-93
CODEN: ANYAA9; ISSN: 0077-8923
DOCUMENT TYPE: Journal
LANGUAGE: English

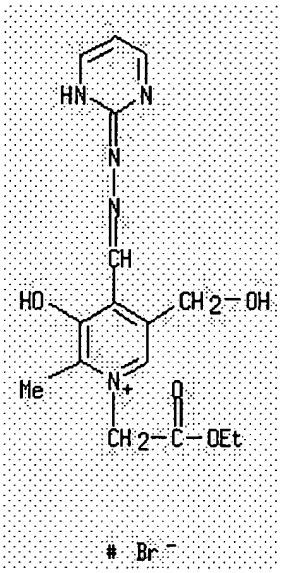
AB A comparative study of the non-iron-overloaded, bile duct-cannulated rat and of the Cebus monkey as iron-clearance models is presented. The ability of desferrioxamine, desferrithiocin, and a pyridoxal isonicotinoyl hydrazone (PIH) analog to clear the metal from these 2 animals is evaluated. Data suggest that although rodents represent a viable first-line animal screen, there is no strict correspondence between the effectiveness of a chelator in rodents and that in primates. Rodent data should be interpreted carefully as it relates to potential human trials. Iron-loading response, the similarity between multiple human and Cebus

serum and hematol. values, and the ability to easily observe changes in behavioral patterns clearly render the Cebus monkey the best preclin. screen.

IT **124050-83-5**, CGP 43902B
RL: BIOL (Biological study)
(iron clearance by, monkey and rodent animal models in evaluation of)

RN 124050-83-5 HCAPLUS

CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyrimidinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



L13 ANSWER 13 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | More References

ACCESSION NUMBER: 1991:199146 HCAPLUS
DOCUMENT NUMBER: 114:199146
TITLE: Iron(II)-chelates based on redox-active pyridoxal-betaines as C-centered radicals causing single- and double-strand scissions to DNA
AUTHOR(S): Iheanacho, Eugene N.; Sarel, Shalom; Samuni, Amram; Avramovici-Grisaru, Shelly; Spira, Dan T.
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Free Radical Research Communications (1991), 11(6), 307-15
CODEN: FRRCEX; ISSN: 8755-0199
DOCUMENT TYPE: Journal
LANGUAGE: English

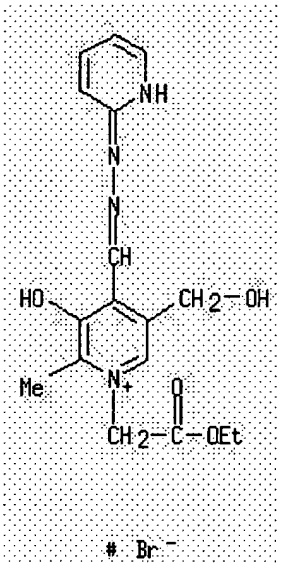
AB The ability of 1-[N-ethoxycarbonylmethylpridoxylidenium]-2-[2'-pyridyl]hydrazine bromide code name [L2-9 = L+, X-]-FE(II) chelate [L2-9-Fe(II)], to induce breaks both in the 43kb linear double-strand λ phage DNA and in the 4363 base pair supercoiled pBR322 plasmid DNA is described. Neither the free ligand nor FE(II) alone demonstrated any effect on the DNA. The cleaving ability occurs instantaneously under strictly anaerobic conditions, either in the presence or absence of catalase. It is also dose dependent. Thus, at λ-DNA:L2-9-Fe(II) molar ratio of 3.7:1.0, the linear DNA is randomly cleaved into fragments ranging from 23.1 kb to 4.3 kb, whereas at approx. 1:1 molar ratio, the range extends down to 2.5 kb fragments. By contrast, at 1:2.7 [plasmid DNA]:chelate-Fe(II) molar ratio, a single-strand nick was obsd., and a double-strand break was noted at a 1:50 ratio ([plasmid

DNA]:chelate-Fe(II). A multistage redox cycling involving a carbon-centered (L,X-)-Fe(III) radical capable of transferring an electron to the DNA to form high unstable [DNA)-. anion-radical is invoked to explain the degrdn. of the chain macromol. Possible modes for regeneration of the chelate-Fe(III) radical both at the cell-free and at the cell levels are proposed.

IT **124076-31-9D**, iron complexes
RL: BIOL (Biological study)
(DNA breakage by)

RN 124076-31-9 HCAPLUS

CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyridinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



L13 ANSWER 14 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | More References

ACCESSION NUMBER: 1990:607346 HCAPLUS
DOCUMENT NUMBER: 113:207346
TITLE: Functionalized bilayer membranes as artificial tryptophan synthase. Characterization of catalytic efficiency, substrate specificity, and reaction selectivity
AUTHOR(S): Murakami, Yukito; Kikuchi, Junichi; Hisaeda, Yoshio; Nakamura, Koichiro; Kitazaki, Tomoyuki; Kaya, Hidenori
CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1990), 63(8), 2339-45
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:207346

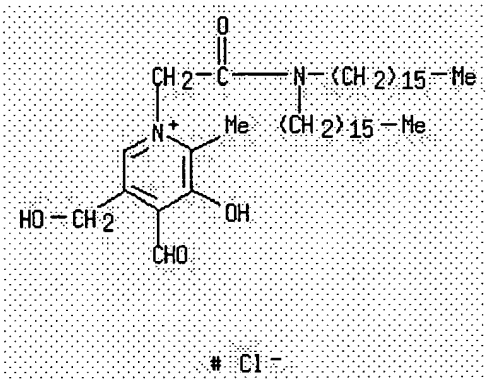
AB Functionalized bilayer membranes having vitamin B6 activity effectively catalyzed β-replacement reactions of serine with indoles to afford the corresponding tryptophan derivs. in aq. media under mild conditions. Catalytic capability of the present artificial enzyme was subjected to change by changing a combination of mol. components constituting the catalyst system. The structural mode of a hydrophobic pyridoxal deriv. as the coenzyme model, the catalytic ability of an amino acid residue placed in a peptide lipid which forms single-walled bilayer vesicles as the

apoenzyme model, and the coordination property of added metal ions were found to be responsible for the overall catalytic performance. Multifunctional assistance was obsd. in the β-replacement reaction of serine with indole, and the reaction proceeded in preference to other side reactions, such as β-elimination, dealdolation, and transamination reactions. Substrate selectivity was found to be primarily dependent on the nucleophilicity of indole derivs.

IT **95930-24-8**
RL: BIOL (Biological study)
(bilayer membranes contg. peptide hydrophobic derivs. and, as tryptophan synthase model)

RN 95930-24-8 HCAPLUS

CN Pyridinium, 1-[2-(dihexadecylamino)-2-oxoethyl]-4-formyl-3-hydroxy-5-(hydroxymethyl)-2-methyl-, chloride (9CI) (CA INDEX NAME)



L13 ANSWER 15 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1990:548739 HCAPLUS
DOCUMENT NUMBER: 113:148739
TITLE: Inhibition of Plasmodium falciparum growth by a synthetic iron chelator
AUTHOR(S): Iheanacho, Eugene N.; Samuni, Amram; Avramovici-Grisaru, Schelly; Sarel, Shalom; Spira, Dan T.
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Transactions of the Royal Society of Tropical Medicine and Hygiene (1990), 84(2), 213-16
CODEN: TRSTAZ; ISSN: 0035-9203
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The susceptibility of the chloroquine-resistant malaria parasite P. falciparum (FCR-3) to a pyridoxal-based iron chelator was tested. Ten μM of the chelator 1-[N-ethoxycarbonylmethylpyridoxylidenium]-2-[2'-pyridyl]hydrazine bromide (code name L2-9) effectively inhibited in vitro growth of the parasites. Presatn. of the chelator with either Fe2+ or Fe3+ partially blocked the inhibitory effect. Two h exposure of parasites to 20 μM L2-9 was sufficient to inhibit their growth irreversibly. Desferrioxamine blocked the inhibitory effect of L2-9. The chelator may be acting by generating free radicals in complexing intracellular iron.

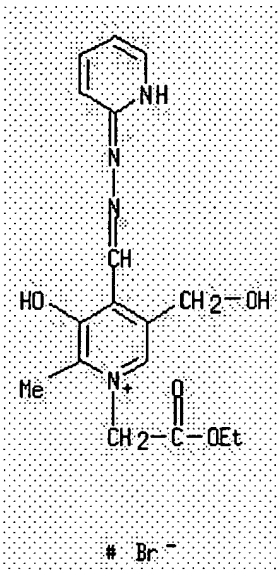
IT **124076-31-9**, L 2-9
RL: BIOL (Biological study)
(Plasmodium falciparum inhibition by)

RN 124076-31-9 HCAPLUS

CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-

)

[(2-pyridinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



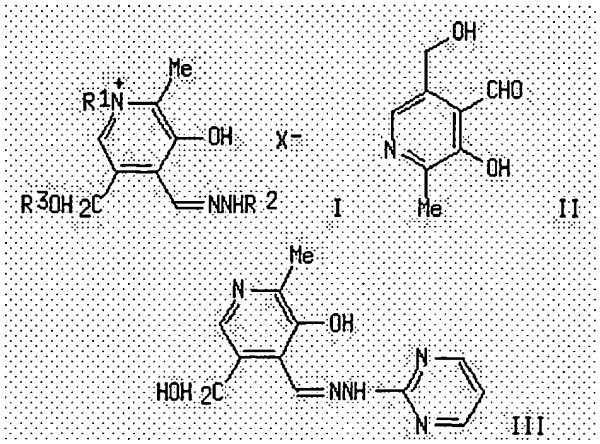
L13 ANSWER 16 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | More References

ACCESSION NUMBER: 1990:98388 HCAPLUS
DOCUMENT NUMBER: 112:98388
TITLE: Preparation of pyridoxal hydrazones as drugs
INVENTOR(S): Sarel, Shalom; Avramovici-Grisaru, Shelly; Hershko, Chaim; Link, Gabriella; Spira, Dan
PATENT ASSIGNEE(S): Yissum Research Development Co., Israel
SOURCE: Eur. Pat. Appl., 16 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 315434	A2	19890510	EP 1988-310314	19881102
EP 315434	A3	19900110		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DK 8806064	A	19890503	DK 1988-6064	19881031
AU 8824637	A1	19890504	AU 1988-24637	19881102
JP 01199946	A2	19890811	JP 1988-278525	19881102
PRIORITY APPLN. INFO.:			IL 1987-84331 A	19871102

GI

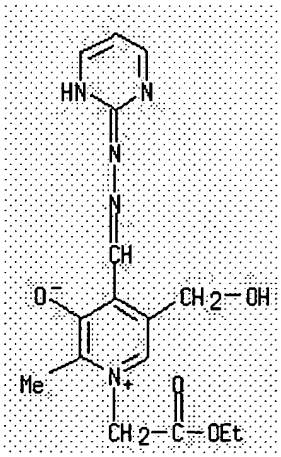


AB Title compds. I [R1 = H, alkyl, CHCO2Me, CH2CO2Et; X = halo, OH; R2 = (oxo-, OH-, NO2-, NH2-, cyano-, CF3-, alkyl-, or alkoxy-substituted) four to seven-membered heterocyclyl having ?1 N, S, or O in the ring; R3 = H, Ac, propionyl, succinyl], useful for treating iron overload, malaria, hepatoma, melanoma, and carcinoma, are prepd. from pyridines II or III (Z = N). A soln. of 2-hydrazinopyrimidine in EtOH was successively treated with II.HCl and aq. NaOH to give III, which was refluxed with BrCH2CO2Et in EtOH to afford I (R1 = CH2CO2Et; R2 = 2-pyrimidyl; R3 = H; X = Br). The latter I (10 mg) and 59Fe tracer was injected s.c. in rats to show 4.2 ? 0.2, 2.9 ? 0.2, 28.9 ? 1.0, and 67.3 ? 2.4% 59Fe in blood, liver, urine, and feces, vs. 27.4 ? 1.6, 12.1 ? 0.6, 0.1 ? 0, and 3.1 ? 0% for control.

IT **124050-81-3P 124050-83-5P 124076-31-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as pharmaceutical)

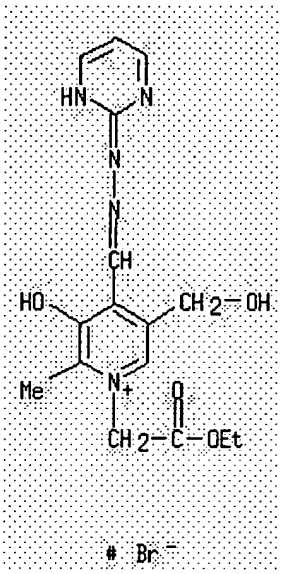
RN 124050-81-3 HCAPLUS

CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyrimidinylhydrazono)methyl]-, inner salt (9CI) (CA INDEX NAME)

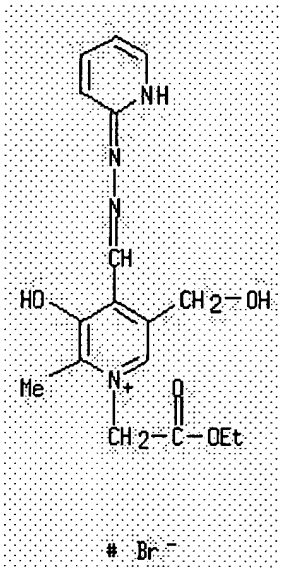


RN 124050-83-5 HCAPLUS

CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyrimidinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



RN 124076-31-9 HCAPLUS
CN Pyridinium, 1-(2-ethoxy-2-oxoethyl)-3-hydroxy-5-(hydroxymethyl)-2-methyl-4-[(2-pyridinylhydrazono)methyl]-, bromide (9CI) (CA INDEX NAME)



L13 ANSWER 17 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1988:434426 HCAPLUS
DOCUMENT NUMBER: 109:34426
TITLE: Functionalized bilayer membranes as artificial transaminase: modification of the active site and its consequence in catalytic efficiency
AUTHOR(S): Murakami, Yukito; Kikuchi, Junichi; Akiyoshi, Kazunari; Shiratori, Nobuyuki
CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Israel Journal of Chemistry (1988), Volume Date 1987, 28(1), 23-8
CODEN: ISJCAT; ISSN: 0021-2148
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The transamination reaction of L-phenylalanine with pyruvate as catalyzed

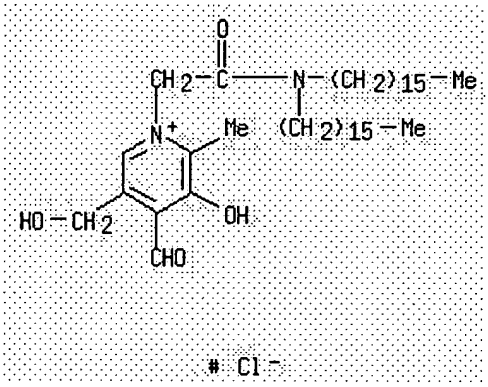
by the artificial transaminase formed with synthetic bilayer aggregates was examd. in aq. media under mild kinetic conditions. Each catalyst system was constructed with a combination of a synthetic peptide lipid, a hydrophobic vitamin B6 deriv., and metal ions. The modification of the active site in the present artificial transaminase was performed by changing a combination of mol. components constituting the catalytic system. Whereas the catalytic activity was scarcely influenced by differences in aggregate structure, bilayer type (single- or multi-walled), and Cu(II) concn., mol. structures of the hydrophobic vitamin B6 and an amino acid residue of the peptide lipid had significant effects on the reactivity.

IT **95930-24-8**

RL: BIOL (Biological study)
(in artificial phenylalanine transaminase, enzyme catalytic efficiency in relation to)

RN 95930-24-8 HCAPLUS

CN Pyridinium, 1-[2-(dihexadecylamino)-2-oxoethyl]-4-formyl-3-hydroxy-5-(hydroxymethyl)-2-methyl-, chloride (9CI) (CA INDEX NAME)



L13 ANSWER 18 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1988:419379 HCAPLUS
DOCUMENT NUMBER: 109:19379
TITLE: Functionalized bilayer membranes having vitamin B6 activity as artificial tryptophan synthase
AUTHOR(S): Murakami, Yukito; Kikuchi, Junichi; Kitazaki, Tomoyuki
CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Journal of the Chemical Society, Chemical Communications (1988), (2), 143-5
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English

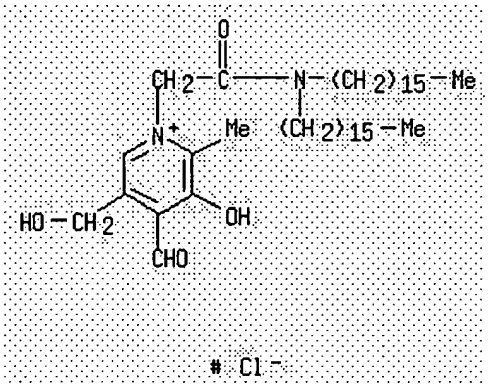
AB Synthetic bilayer vesicles having vitamin B6 activity markedly enhanced the β-replacement reaction of serine with indole to afford tryptophan, showing turnover behavior, in aq. media under mild conditions.

IT **95930-24-8P**

RL: PREP (Preparation)
(bilayer membrane contg. lipopeptide and, tryptophan formation by serine reaction with indole enhancement by)

RN 95930-24-8 HCAPLUS

CN Pyridinium, 1-[2-(dihexadecylamino)-2-oxoethyl]-4-formyl-3-hydroxy-5-(hydroxymethyl)-2-methyl-, chloride (9CI) (CA INDEX NAME)



L13 ANSWER 19 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

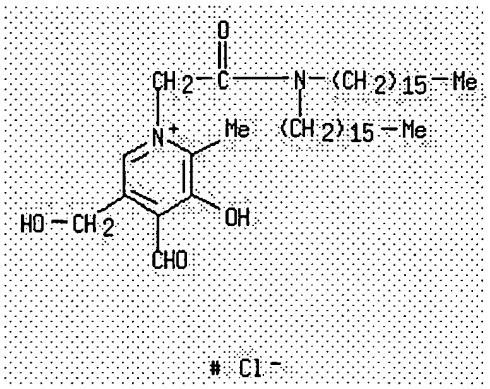
Full Text | Citing References

ACCESSION NUMBER: 1987:478210 HCAPLUS
DOCUMENT NUMBER: 107:78210
TITLE: Kinetics and mechanism of transamination reaction of L-phenylalanine with hydrophobic pyridoxal in vesicular and micellar phases
AUTHOR(S): Murakami, Yukito; Kikuchi, Junichi; Akiyoshi, Kazunari; Imori, Toru
CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1986), (9), 1445-52
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:78210

AB A hydrophobic pyridoxal deriv. quaternized at the pyridyl nitrogen with a double-chain segment (PL+2C16) was embedded in the single-walled vesicle of N,N-dihexadecyl-Nα-[6-(trimethylammonio)hexanoyl]-L-alaninamide bromide (N+C5Ala2C16), and the pyridoxal moiety was fixed in the hydrogen-belt domain of the vesicle. While the transamination of L-phenylalanine (L-Phe), a hydrophobic α-amino acid, with PL+2C16 in the vesicle and the hexadecyltrimethylammonium bromide (CTAB) micelle proceeded slowly to afford the pyridoxamine deriv. (PM+2C16) and β-phenylpyruvic acid, addn. of metal ions to the equil. mixt. of the aldimine Schiff's base (ASB), PL+2C16, and L-Phe caused acceleration of the overall transamination rate. The transamination was most effectively catalyzed by copper(II) ions in the N+C5Ala2C16 vesicle and the CTAB micelle. The catalytic activity of copper(II) ions was so enhanced as to allow significant accumulation of the carbanion chelate, derived from the ASB chelate by α-hydrogen removal, as an intermediate in the aldimine-ketimine isomerization. The reactivity of the overall copper(II)-catalyzed transamination was greater in the vesicle than in the micelle and primarily controlled by the collapse ratio of the copper(II)-carbanion species as clarified by detailed kinetic anal.

IT **95930-24-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and transamination reaction of, with phenylalanine in vesicular and micellar phases)

RN 95930-24-8 HCAPLUS
CN Pyridinium, 1-[2-(dihexadecylamino)-2-oxoethyl]-4-formyl-3-hydroxy-5-(hydroxymethyl)-2-methyl-, chloride (9CI) (CA INDEX NAME)



L13 ANSWER 20 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

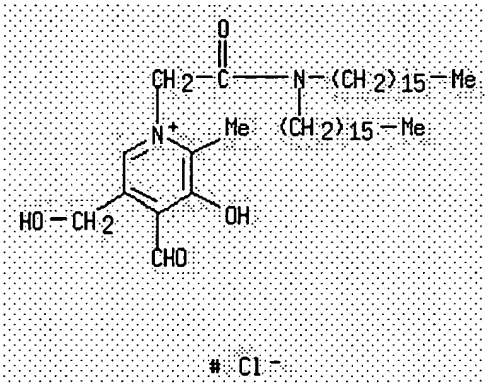
Full Text | Cited References

ACCESSION NUMBER: 1986:168799 HCAPLUS
DOCUMENT NUMBER: 104:168799
TITLE: Functionalized bilayer vesicle as a catalyst for transamination: artificial transaminase
AUTHOR(S): Murakami, Yukito; Kikuchi, Junichi; Akiyoshi, Kazunari; Imori, Toru
CORPORATE SOURCE: Dep. Org. Synth., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1985), (12), 1919-24
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The nonenzymic transamination reaction of α-amino acids with α-keto acids was studied in aq. medium at 30?. The functionalized single-walled covesicle composed of a synthetic peptide lipid, N,N-dihexadecyl-Nα-[6-(trimethylammonio)hexanoyl]-L-histidinamide bromide, and a hydrophobic pyridoxal deriv., 1-(N,N-dihexadecylcarbamoylmethyl)-2-methyl-3-hydroxy-4-formyl-5-(hydroxymethyl)pyridinium chloride, effectively catalyzed amino group transfer from L-phenylalanine to pyruvic acid in the presence of Cu(II) ions, showing turnover behavior. The catalytic activity of the vesicular system was much higher than those of 1,2-dimethyl-3-hydroxy-4-formyl-5-(hydroxymethyl)pyridinium chloride and pyridoxal examd. in aq. media contg. Cu(II) ions. The rate-detg. step involved in the catalytic cycle involving the vesicular catalyst is primarily assigned to the product-releasing process, the hydrolysis of the Cu(II) chelate of the aldimine Schiff's base to afford alanine.

IT **95930-24-8**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, in bilayer vesicles with copper(II) ions and synthetic peptide lipid, for transamination of amino acids with keto acids)

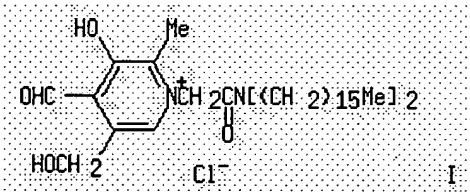
RN 95930-24-8 HCAPLUS
CN Pyridinium, 1-[2-(dihexadecylamino)-2-oxoethyl]-4-formyl-3-hydroxy-5-(hydroxymethyl)-2-methyl-, chloride (9CI) (CA INDEX NAME)



L13 ANSWER 21 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

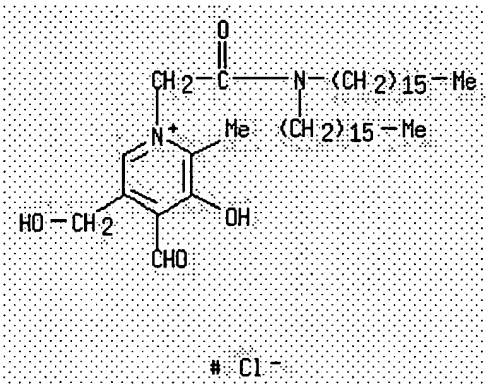
ACCESSION NUMBER: 1985:167129 HCAPLUS
DOCUMENT NUMBER: 102:167129
TITLE: Transamination reaction of hydrophobic pyridoxal with an α-amino acid in functionalized bilayer vesicles: cooperative catalysis by the imidazolyl group and copper(II) ions
AUTHOR(S): Murakami, Yukito; Kikuchi, Junichi; Imori, Toru; Akiyoshi, Kazunari
CORPORATE SOURCE: Dep. Org. Synth., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Journal of the Chemical Society, Chemical Communications (1984), (21), 1434-5
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The hydrophobic pyridoxal deriv. I underwent transamination with L-phenylalanine in single-walled bilayer vesicles formed from Me3N+(CH2)5CONHCRHCON[(CH2)15Me]2 Br- (R = Me, 4-imidazoylmethyl). The reaction proceeds through the fast equilibrated formation of an aldimino Schiff base intermediate followed by much slower conversion into the pyridoxamine deriv. and β-phenylpyruvate. Coordination of Cu2+ to the intermediate caused a marked rate acceleration.

IT **95930-24-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and transamination of, with phenylalanine in bilayer vesicles, kinetics of,)

RN 95930-24-8 HCAPLUS
CN Pyridinium, 1-[2-(dihexadecylamino)-2-oxoethyl]-4-formyl-3-hydroxy-5-(hydroxymethyl)-2-methyl-, chloride (9CI) (CA INDEX NAME)



L13 ANSWER 22 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

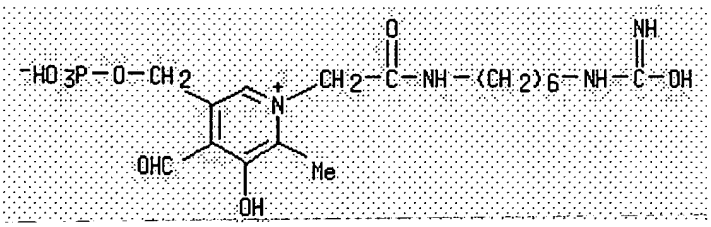
ACCESSION NUMBER: 1979:504494 HCAPLUS
DOCUMENT NUMBER: 91:104494
TITLE: Immobilization of pyridoxal 5'-phosphate and pyridoxal 5'-phosphate-dependent enzymes on Sepharose
AUTHOR(S): Ikeda, Seiichiro; Fukui, Saburo
CORPORATE SOURCE: Dep. Biochem., Ohio State Univ., Columbus, OH, USA
SOURCE: Methods in Enzymology (1979), 62(Vitam. Coenzymes, Part D), 517-27
CODEN: MENZAU; ISSN: 0076-6879
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Three types of Sepharose-bound pyridoxal 5'-phosphate (I) were prepd. by coupling diazotized p-aminobenzamidohexyl-Sepharose to the 6-position of I or coupling to bromoacetamidohexyl-Sepharose to yield the N- and 3-O-immobilized I derivs. The properties of the I-Sepharose derivs. are characterized and they are applied to the affinity chromatog. of apo-tryptophanase from Escherichia coli and for the immobilization of I-dependent enzymes through biospecific binding to the active center.

IT **71244-18-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and properties of)
RN 71244-18-3 HCAPLUS
CN Agarose, [6-[[[4-formyl-3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridinio]acetyl]amino]hexyl]carbamimidate, inner salt (9CI) (CA INDEX NAME)

CM 1

CRN 173450-93-6
CMF C17 H27 N4 O8 P



CM 2

CRN 9012-36-6
CMF Unspecified

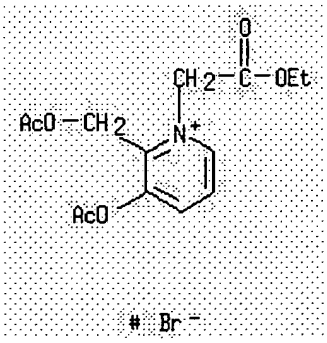
CCI PMS, MAN

STRUCTURE DIAGRAM IS NOT AVAILABLE

L13 ANSWER 23 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1972:419499 HCAPLUS
DOCUMENT NUMBER: 77:19499
TITLE: Indolizines. II. Facile synthesis of 3-alkoxycarbonyl-, 3-cyano-, and 3-carbamoylindolizines and its mechanism
AUTHOR(S): Dainis, I.
CORPORATE SOURCE: Chem. Sch., Univ. New South Wales, Kensington, Australia
SOURCE: Australian Journal of Chemistry (1972), 25(5), 1025-50
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Acylative cyclization of 2-methylpyridinium (I, R = CN, CO2R1, Me, CH(:NOH) gave 2,3-disubstituted and 1-acyl-2,3-disubstituted indolizines, e.g., II (R1 = Ph, CO2Et, CN, CONH2, CO2H, CO2CH2Ph, CH:NOH, R2 = Me, Et, Ph). This method provided indolizines bearing electroneg. 3-substituents. With 2-substituted pyridinium salts this method provided 1-acetoxy-2,3-disubstituted and other 1,2,3-trisubstituted indolizines. Hydroxypyridines gave acetoxyindolizines. Product studies showed that acyl- and diacylmethines were the major intermediates. Treatment of indolizines with ClCO2Et gave Et indolizine-3-carboxylates. These products and also 3-cyanoindolizines were characterized by reaction with acid formaldehyde to give methylene-1,1'-diindolizines.
IT **36827-04-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 36827-04-0 HCAPLUS
CN Pyridinium, 3-(acetyloxy)-2-[(acetyloxy)methyl]-1-(2-ethoxy-2-oxoethyl)-, bromide (9CI) (CA INDEX NAME)



L13 ANSWER 24 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

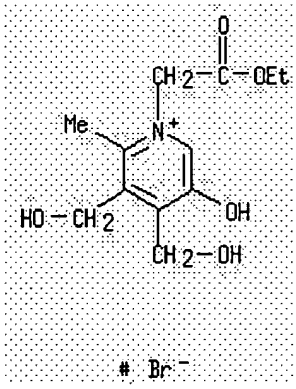
Full Text | Citing References

ACCESSION NUMBER: 1966:438420 HCAPLUS
DOCUMENT NUMBER: 65:38420
ORIGINAL REFERENCE NO.: 65:7136g-h
TITLE: Polyfluoroalkylation. The nucleophilic equivalent of Friedel-Crafts reactions
AUTHOR(S): Chambers, R. D.; Storey, R. A.; Musgrave, W. K. R.

CORPORATE SOURCE: Univ. Sci Labs., Durham, UK
SOURCE: Chemical Communications (London) (1966), (12), 384-5
CODEN: CCOMA8; ISSN: 0009-241X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 65:38420

AB Fluoro olefins are known to react with F- in aprotic solvents and there is an analogy between the role of F- in fluorocarbon chemistry and H+ in hydrocarbon chemistry. This makes possible the nucleophilic equiv. of Friedel-Crafts reactions involving a fluoro olefin and a polyfluoroaromatic compd. in the presence of F-:F- + CF2:CR2 ? CF3C-R2 + ArF ? ArCR2CF3 + F-. Pentafluoropyridine, CF3CF:CF2 (I), and KF in sulfolane react to give the resp. 2,4-disubstituted (5%) and the 4-monosubstituted (90%) products. C6F3NO2 with I gave mainly the 4-mono (30%) and the 2,4-disubstituted (30%) products. By-products were formed by displacement of the NO2 group.

IT **6600-97-1**, Picolinium, 1-(carboxymethyl)-5-hydroxy-3,4-bis(hydroxymethyl)-2-, bromide, Et ester
(prepn. of)
RN 6600-97-1 HCAPLUS
CN 2-Picolinium, 1-(carboxymethyl)-5-hydroxy-3,4-bis(hydroxymethyl)-, bromide, ethyl ester (8CI) (CA INDEX NAME)



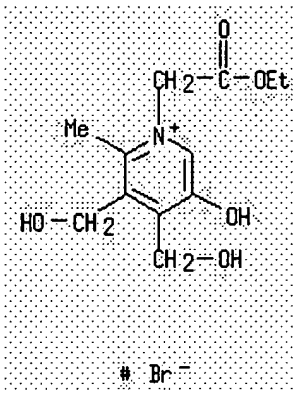
L13 ANSWER 25 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1966:438419 HCAPLUS
DOCUMENT NUMBER: 65:38419
ORIGINAL REFERENCE NO.: 65:7136g
TITLE: Arylazo derivatives of pyridoxine
AUTHOR(S): Katritzky, A. R.; Kucharska, H. Z.; Tucker, M. J.; Wuest, H. M.
CORPORATE SOURCE: Univ. East Anglia, Norwich, UK
SOURCE: Journal of Medicinal Chemistry (1966), 9(4), 620-2
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of five 6-arylazopyridoxine HCl salts were synthesized. These compds. exhibited no significant in vivo inhibition of Sarcoma 180 tumors.

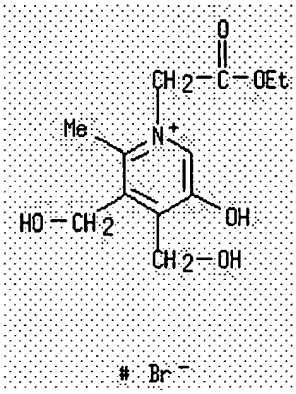
IT **6600-97-1**, Picolinium, 1-(carboxymethyl)-5-hydroxy-3,4-bis(hydroxymethyl)-2-, bromide, Et ester
(prepn. of)
RN 6600-97-1 HCAPLUS
CN 2-Picolinium, 1-(carboxymethyl)-5-hydroxy-3,4-bis(hydroxymethyl)-, bromide, ethyl ester (8CI) (CA INDEX NAME)



L13 ANSWER 26 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1966:438418 HCAPLUS
DOCUMENT NUMBER: 65:38418
ORIGINAL REFERENCE NO.: 65:7136d-g
TITLE: Reaction of aryl ketones with cyclopentadienyl sodium. Syntheses of fulvenylmethanols
AUTHOR(S): Mohrbacher, R. J.; Paragamian, V.; Carson, E. L.; Puma, B. M.; Rasmussen, C. R.; Meschino, J. A.; Poos, G. I.
CORPORATE SOURCE: Dept. of Chem. Res., McNeil Labs., Inc., Fort Washington, PA
SOURCE: Journal of Organic Chemistry (1966), 31(7), 2149-59
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The reaction of 2-benzoylpyridine with cyclopentadienylsodium in alc. can be directed to give the expected 6-phenyl-6-(2-pyridyl)fulvene (I) as its dimer in 88% yield or the novel α phenyl-α-[6-phenyl-6-(2-pyridyl)-2-fulvenyl]-2-pyridinemethanol (II) in 86% yield by varying the conditions. The reaction conditions which favor formation of I or II are discussed in terms of a mechanism for their formation. A variety of diaryl and alkyl aryl ketones, in which the aryl groups were Ph, substituted phenyl, 2-, 3-, or 4-pyridyl, thienyl, or quinolyl, were allowed to react with cyclopentadienylsodium. Strongly electroneg. aryl groups are required for conversion of diaryl ketones to 2-fulvenylmethanols. Aryl 2- (or 4-) pyridyl and di-2- (or 4-) pyridyl ketones form 2-fulvenylmethanols readily. Most diphenyl ketones do not form 2-fulvenylmethanols readily and alkyl pyridyl ketones give only trace amts. of fulvenylmethanols.
IT **6600-97-1**, Picolinium, 1-(carboxymethyl)-5-hydroxy-3,4-bis(hydroxymethyl)-2-, bromide, Et ester
(prepn. of)
RN 6600-97-1 HCAPLUS
CN 2-Picolinium, 1-(carboxymethyl)-5-hydroxy-3,4-bis(hydroxymethyl)-, bromide, ethyl ester (8CI) (CA INDEX NAME)



L13 ANSWER 27 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1962:66960 HCAPLUS
DOCUMENT NUMBER: 56:66960
ORIGINAL REFERENCE NO.: 56:12910i,12911a-f
TITLE: Carboxylic acid amides of N-aminoalkyleneheterocyclic amines
INVENTOR(S): McCabe, John J., Jr.; Mannheimer, Hans S.
SOURCE: Continuation-in-part of U.S. 3,001,996. (CA 56, 10052b)
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3001997		19610926	US 1960-20258	19600406
PRIORITY APPLN. INFO.:			US	19600406

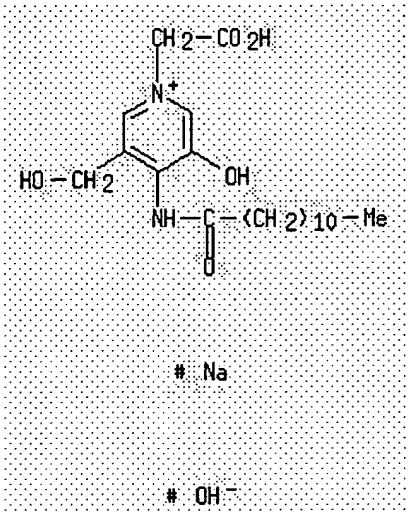
GI For diagram(s), see printed CA Issue.

AB Straight-chain, org. monocarboxylic acids (C5-19) react with heterocyclic di- and triamines to give the title compds., useful as H2O-sol., amphoteric, nontoxic, nonvesicant surface-active substances with fungicidal and bactericidal properties. Laurie acid 200 and 4-(2-aminoethyl)-morpholine 131 is heated to 170? during 3 hrs. at 110 mm. to remove H2O 18, let cool to room temp., added to ClCH2CO2H 96, NaOH 80, and H2O 300 parts at 20?, the mixt. heated to 95?, and held there while the pH is lowered from 13 to 8-8.5 to obtain a clear aq. soln. of C11H23CONHCH2 CH2(HO)(NaO2CCH2)Z (Z = morpholinium). Prepd. similarly are aq. solns. of the following: C9H19CONHCH2CH2(HO)(NaO2CCH2CH2)Z (Z = piperidinium),C5H11CONHCH2CH2(HO)(NaO2CCH2)OCH2CH2)Z (Z = 2-pyrrolinium), C17H35CONHCH2CH2(HO) [NaO2CCH(OH)CH2O-CH2CH2]Z (Z = pyrrolidinum), C11H23CONHC5H4N(CH2CO2Na)OH, C11H23CONHCH2CH2(HO)(NaO2CCH2)Z (Z = 2,4-dimethyl-3-ethylpyrrolium), and I-XI].

IT **106655-59-8**, Pyridinium, 1-(carboxymethyl)-3-hydroxy-5-(hydroxymethyl)-4-lauramido-, hydroxide, Na salt
(prepn. of)

RN 106655-59-8 HCAPLUS

CN 1-(Carboxymethyl)-3-hydroxy-5-(hydroxymethyl)-4-lauramidopyridinium hydroxide, sodium salt (7CI) (CA INDEX NAME)



L13 ANSWER 28 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1946:20771 HCAPLUS
DOCUMENT NUMBER: 40:20771
ORIGINAL REFERENCE NO.: 40:4065c-i
TITLE: Chemical treatment of tumors. XII. Some quaternary ammonium salts of heterocyclic bases
AUTHOR(S): Hartwell, Jonathan L.; Kornberg, Sylvia R. L.
CORPORATE SOURCE: U.S. Pub. Health Service, Bethesda, MD
SOURCE: Journal of the American Chemical Society (1946), 68, 868-70
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

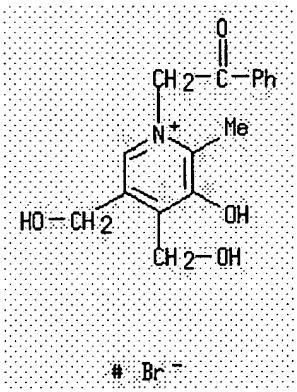
AB cf. C.A. 40, 68.9. The iodides were prepd. by the method of King (C.A. 38, 3981.1; 40, 3417.5), i.e., by the action of iodine and a base upon an arom. ketone. The bromides were prepd. from RCOCH2Br and the amine by warming on the water bath up to 30 min. or from PhCH2CH2Br with 20% excess of amine and heating for periods of 45 min. to 16 h. Perchlorates were prepd. from the bromides by the action of 50% excess of HClO4; in general the iodides did not react with HClO4. All m.ps. are cor. In the following, the amine used and the halide obtained, the m.p., and the yield of crude compd. are given. Phenacyl derivs.: pyridine, iodide, 215-16? (decompn.), 84% (oxime, m. 166.7-8.3?, 97%); 2-picoline, iodide, cream, 206.4-7.1? (decompn.), 8%; 3-picoline, iodide, light yellow, 183.7-4.7?, 29%; 4-picoline, bromide, 261.2-1.8? (decompn.), 67%; iodide, buff, 201.1-1.9? (decompn.), 36%; perchlorate, pale yellow, 175.4-6.1?, 100% (on basis of bromide); nicotinamide, bromide, pale yellow, 235.8-8.2?, 90%; pyridoxine, bromide, pale yellow, 208-10? (decompn.), 44%; quinoline, bromide, pale yellow, 191-2.6?, 68%; isoquinoline, iodide, yellow, 178.7-80?, 40%; 3-methylisoquinoline, iodide, yellow, 199-9.7? (decompn.), 56%. p-Methoxyphenacyl derivs.: pyridine, iodide, light yellow, 211.5-14.5? (decompn.), 79% (oxime, with 0.5 mol. H2O, 113.4-15?, 57%); perchlorate, yellow, 201-2.2?, 87% (on basis of iodide); 2-picoline, iodide, buff, 204.9-5.9? (decompn.), 9%; 3-isomer, light pink, 202.3-3.5?, 57%; 4-isomer, pink 230.8-2.2?, 8%; quinoline, bromide, with 1 mol. H2O, yellow, 227.3-8.5? (decompn.), 49%; perchlorate, pink, 224.7-6.4? (decompn.), 87% (on basis of bromide); isoquinoline, iodide, yellow, 234.7-5.7?, 58%; 3-methylisoquinoline, iodide,

yellow, 225.7-6.9? (decompn.), 57%. 2-Phenylethyl derivs.: pyridine, bromide, 125.9-6.5?, 89%; 2-picoline, bromide, 198.1-8.9?, 93%; 3-isomer (I), 123.3-7.5?, 100%; 4-isomer, with 2/3 mol. H2O, 88.8-91?, 76%; perchlorate, 126.9-7.5?, 28% (on basis of bromide); quinoline, bromide, cream, 127.3-8.3?, 84%; isoquinoline, bromide, with 4/3 mols. H2O, buff, 72.7-3.9?, 80%; perchlorate, 170.4-1.1?, 100%; 3-methylisoquinoline, bromide, 249-50.2? (decompn.), 84%. In the prepn. of I, it is necessary to reflux the reactants in EtOH for 48 h.; otherwise compd. m. 109-10? results, which does not contain ionizable Br; I is quite labile and yields the lower-melting compd. on crystn.; in an attempt to prep. the perchlorate, the same compd. was formed. 1-(2-Naphthacyl)pyridinium iodide, light yellow, 217-17.8? (decompn.), 85% (oxime, pale yellow, 203-5? (decompn.), 63%). β-Bromostyrene gave too small yields of products for the reaction to be useful.

IT **6273-67-2**, Pyridinium, 3-hydroxy-4,5-bis(hydroxymethyl)-2-methyl-1-phenacyl-, bromide
(prepn. of)

RN 6273-67-2 HCAPLUS

CN Pyridinium, 3-hydroxy-4,5-bis(2-hydroxymethyl)-2-methyl-1-(2-oxo-2-phenylethyl)-, bromide (9CI) (CA INDEX NAME)



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L3          17 S L1 FULL

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L5           9 S L4 AND HOFMANN, T?/AU

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L16          0 S L13 AND FRANK, O?/AU
L17          0 S L13 AND SOLDO, T?/AU
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L19          0 S L13 AND VILLARD, R?/AU
L20          0 S L13 AND ROBERT, F?/AU

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=> s l12
L21          2 L12

=> d l21, all, 1-2

L21  ANSWER 1 OF 2  CAOLD  COPYRIGHT 2006 ACS on STN
AN   CA65:7136g  CAOLD
TI   arylazo derivs. of pyridoxine
AU   Katritzky, Alan R.; Kucharska, H. Z.; Tucker, M. J.; Wuest, H. M.
TI   polyfluoroalkylation-nucleophilic equiv. of Friedel-Crafts reactions
AU   Chambers, Richard D.; Storey, R. A.; Musgrave, W. K. R.
IT   6586-24-9   6600-90-4   6600-91-5   6600-92-6   6600-93-7   6600-94-8
     6600-95-9   6600-96-0   6600-97-1   6734-19-6

L21  ANSWER 2 OF 2  CAOLD  COPYRIGHT 2006 ACS on STN
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Full Text

AN CA56:12910i CAOLD
TI carboxylic acid amides of N-aminoalkylene-heterocyclic amines
AU Mannheimer, Hans S.
DT Patent
TI carboxylic acid amides of N-aminoalkyleneheterocyclic amines
AU McCabe, John J., Jr.; Mannheimer, H. S.
DT Patent

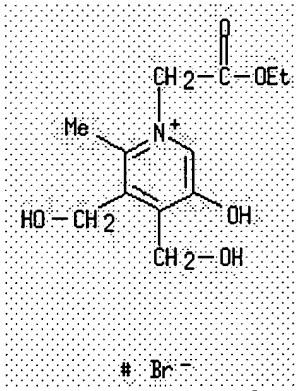
PATENT NO.	KIND	DATE
US 3001997		1961

IT 1748-49-8 13519-23-8 91762-67-3 92853-98-0 93256-67-8 97525-31-0 97771-83-0 98068-21-4 98882-10-1 99997-21-4 99997-23-6 100104-67-4 100268-66-4 100270-91-5 101296-40-6 101378-66-9 103535-49-5 106169-36-2 106336-45-2 **106655-59-8** 106655-63-4 107278-80-8

=> fil reg; d acc 6600-97-1; fil CAOLD

FILE 'REGISTRY' ENTERED AT 14:02:30 ON 10 MAY 2006

ANSWER 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN 6600-97-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Picolinium, 1-(carboxymethyl)-5-hydroxy-3,4-bis(hydroxymethyl)-, bromide, ethyl ester (8CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-(Carboxymethyl)-5-hydroxy-3,4-bis(hydroxymethyl)-2-picolinium bromide, ethyl ester (7CI)
MF C12 H18 N O5 . Br
LC STN Files: CA, CAOLD, CAPLUS
CRN (801154-32-5)



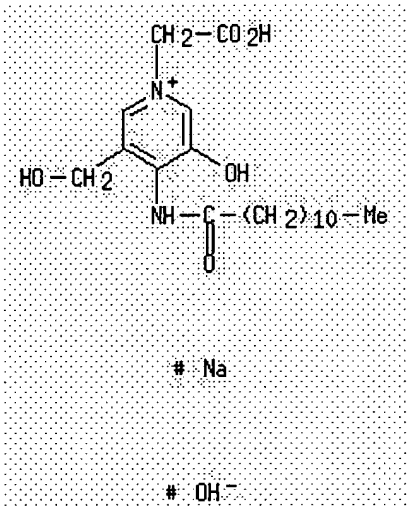
3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 14:02:31 ON 10 MAY 2006

=> fil reg; d acc 106655-59-8; fil CAOLD

FILE 'REGISTRY' ENTERED AT 14:02:34 ON 10 MAY 2006

ANSWER 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN 106655-59-8 REGISTRY
ED Entered STN: 14 Feb 1987
CN 1-(Carboxymethyl)-3-hydroxy-5-(hydroxymethyl)-4-lauramidopyridinium hydroxide, sodium salt (7CI) (CA INDEX NAME)
MF C20 H33 N2 O5 . H O . Na
SR CAOLD
LC STN Files: CA, CAOLD, CAPLUS, TOXCENTER
CRN (803679-75-6)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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